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Figure 1A

Topology diagram of MurI

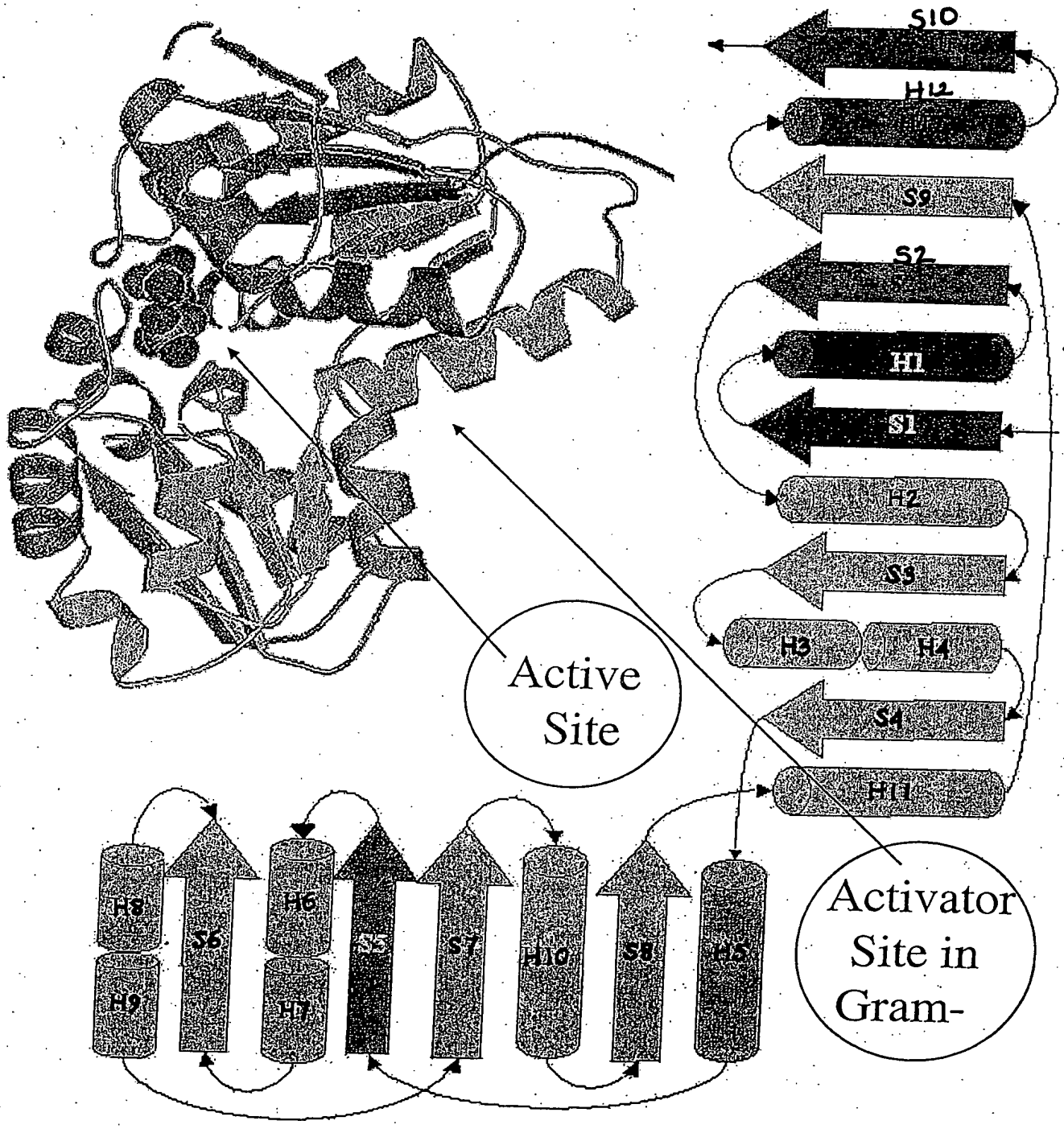


Figure 1B



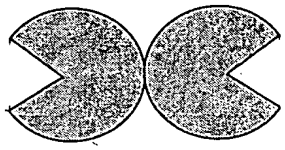
closed form

Figure 1C



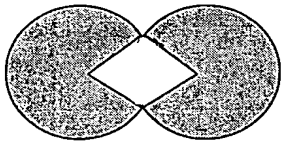
open form

Figure 1D



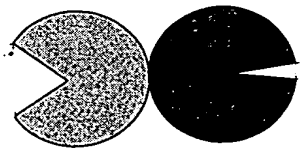
Tail -Tail Dimer

Figure 1E



Head - Head Dimer

Figure 1F



Mixed Forms Dimer

Figure 1G



Activator-modulated monomer

Figure 2A

Structural sequence alignments of MurIs																																	
S	H	All MurIs	MurI-G-	G+	E coli			S. aureus						E. faecalis						E. faecium			H. pylori						A. pyrophilus				
					A chain			A chain			B chain			A chain			B chain			A chain			A chain			B chain			A chain				
																				2	I												
																				3	R												
																				4	L												
														2	S		2	S		5	T												
					20	P		1	M		1	M		3	N	T	3	N	T	6	D												
				1	21	R	E	2	N		2	N		4	Q	T	4	Q	T	7	N												
				1	22	P	E	3	K	S	3	K		5	E	S	5	E	S	8	R		1	M		1	M		1	M			
		1	1	1	23	T	E	4	P		4	P		6	A		6	A		9	P		2	K	E	2	K	E	2	K	E		
S1		1	1	1	24	V	E	5	I	E	5	I	E	7	I	E	7	I	E	10	I	E	3	I	E	3	I	E	3	I	E		
S1		1	1	1	25	L	E	6	G	E	6	G	E	8	G	E	8	G	E	11	G	E	4	G	E	4	G	E	4	G	E		
S1		1	1	1	26	V	E	7	V	E	7	V	E	9	L	E	9	L	E	12	F	E	5	V	E	5	V	E	5	I	E		
S1		1	1	1	27	F	E	8	I	E	8	I	E	10	I	E	10	I	E	13	I	E	6	F	E	6	F	E	6	F	E		
S1		1	1	1	28	D	E	9	D	E	9	D	E	11	D	E	11	D	E	14	D	E	7	D	E	7	D	E	7	D	E		
		1	1	1	29	S	S	10	S	S	10	S	S	12	S	S	12	S	S	15	S	S	8	S	S	8	S	S	8	S	S		
		1	1	1	30	G	S	11	G	S	11	G	S	13	G	S	13	G	S	16	G	S	9	G	S	9	G	S	9	G	S		

Figure 2B

		1	1	1	31	V	S	12	V	S	12	V	S	14	V	S	14	V	S	17	V	S	10	V	S	10	V	S	10	V	S
		1	1	1	32	G	T	13	G	T	13	G	T	15	G	T	15	G	T	18	G	T	11	G	T	11	G	T	11	G	G
		1	1	1	33	G	H	14	G	T	14	G	T	16	G	T	16	G	T	19	G	T	12	G	T	12	G	T	12	G	G
		1	1	1	34	L	H	15	L	H	15	L	H	17	L	H	17	L	H	20	L	H	13	F	H	13	F	H	13	L	G
		1	1	1	35	S	H	16	T	H	16	T	H	18	T	H	18	T	H	21	T	H	14	S	H	14	S	H	14	T	T
	H1	1	1	1	36	V	H	17	V	H	17	V	H	19	V	H	19	V	H	22	V	H	15	V	H	15	V	H	15	V	H
	H1	1	1	1	37	Y	H	18	A	H	18	A	H	20	L	H	20	L	H	23	V	H	16	L	H	16	L	H	16	L	H
	H1	1	1	1	38	D	H	19	K	H	19	K	H	21	K	H	21	K	H	24	K	H	17	K	H	17	K	H	17	K	H
	H1	1	1	1	39	E	H	20	E	H	20	E	H	22	E	H	22	E	H	25	E	H	18	S	H	18	S	H	18	A	H
	H1	1	1	1	40	I	H	21	I	H	21	I	H	23	A	H	23	A	H	26	A	H	19	L	H	19	L	H	19	I	H
	H1	1	1	1	41	R	H	22	M	H	22	M	H	24	L	H	24	L	H	27	L	H	20	L	H	20	L	H	20	R	H
	H1	1	1	1	42	H	H	23	R	H	23	R	H	25	K	H	25	K	H	28	K	H	21	K	H	21	K	H	21	N	H
	H1	1	1	1	43	L	H	24	Q	H	24	Q	H	26	Q	H	26	Q	H	29	Q	H	22	A	H	22	A	H	22	R	H
				1	44	L	S	25	L		25	L		27	L		27	L		30	L		23	R	T	23	R	T	23	Y	S
				1	45	P	T	26	P	T	26	P	T	28	P	T	28	P	T	31	P	T	24	L		24	L		24	R	T
				1	46	D	T	27	N	T	27	N	T	29	N	T	29	N	T	32	N	T	25	F		25	F		25	K	T
				1	47	L	S	28	E		28	E		30	E		30	E		33	E		26	D	S	26	D	S	26	V	
		1	1	1	48	H	E	29	T		29	T		31	R		31	R		34	N		27	E	E	27	E	E	27	D	E
S2		1	1	1	49	Y	E	30	I	E	30	I	E	32	L	E	32	L	E	35	I	E	28	I	E	28	I	E	28	I	E
S2		1	1	1	50	I	E	31	Y	E	31	Y	E	33	I	E	33	I	E	36	L	E	29	I	E	29	I	E	29	V	E

Figure 2C

S2		1	1	1	51	Y	E	32	Y	E	32	Y	E	34	Y	E	34	Y	E	37	F	E	30	Y	E	30	Y	E	30	Y	E
S2		1	1	1	52	A	E	33	L	E	33	L	E	35	L	E	35	L	E	38	V	E	31	Y	E	31	Y	E	31	L	E
S2		1	1	1	53	F	E	34	G	E	34	G	E	36	G	E	36	G	E	39	G	E	32	G	E	32	G	E	32	G	E
		1	1	1	54	D		35	D		35	D		37	D		37	D		40	D		33	D		33	D		33	D	
		1	1	1	55	N	T	36	I	T	36	I	T	38	T	T	38	T	T	41	T	T	34	S	T	34	S	T	34	T	T
		1	1	1	56	V	T	37	G	T	37	G	T	39	A	T	39	A	T	42	A	T	35	A	T	35	A	T	35	A	T
		1	1	1	57	A	T	38	R	T	38	R	T	40	R	T	40	R	T	43	R	S	36	R	T	36	R	T	36	R	T
		1	1	1	58	F		39	C		39	C		41	C		41	C		44	C		37	V		37	V		37	V	
		1	1	1	59	P		40	P		40	P		42	P		42	P		45	P		38	P		38	P		38	P	
		1	1	1	60	Y	T	41	Y		41	Y		43	Y		43	Y		46	Y		39	Y		39	Y		39	Y	
		1	1	1	61	G	T	42	G	T	42	G	T	44	G	T	44	G	T	47	G	T	40	G	T	40	G	T	40	G	T
		1	1	1	62	E	T	43	P	T	43	P	T	45	P	T	45	P	T	48	P	T	41	T	T	41	T	T	41	I	T
		1	1	1	63	K	S	44	R	S	44	R	S	46	R	S	46	R	S	49	R	S	42	K	S	42	K	S	42	R	S
		1	1	1	64	S		45	P		45	P		47	P		47	P		50	P		43	D		43	D		43	S	
	H2	1	1	1	65	E	H	46	G	H	46	G	H	48	A	H	48	A	H	51	A	H	44	P	H	44	P	H	44	K	H
	H2	1	1	1	66	A	H	47	E	H	47	E	H	49	E	H	49	E	H	52	E	H	45	T	H	45	T	H	45	D	H
	H2	1	1	1	67	F	H	48	Q	H	48	Q	H	50	Q	H	50	Q	H	53	Q	H	46	T	H	46	T	H	46	T	H
	H2	1	1	1	68	I	H	49	V	H	49	V	H	51	V	H	51	V	H	54	V	H	47	I	H	47	I	H	47	I	H
	H2	1	1	1	69	V	H	50	K	H	50	K	H	52	V	H	52	V	H	55	I	H	48	K	H	48	K	H	48	I	H
	H2	1	1	1	70	E	H	51	Q	H	51	Q	H	53	Q	H	53	Q	H	56	Q	H	49	Q	H	49	Q	H	49	R	H

Figure 2D

	H2	1	1	1	71	R	H	52	Y	H	52	Y	H	54	F	H	54	F	H	57	Y	H	50	F	H	50	F	H	50	Y	H
	H2	1	1	1	72	V	H	53	T	H	53	T	H	55	T	H	55	T	H	58	T	H	51	G	H	51	G	H	51	S	H
	H2	1	1	1	73	V	H	54	V	H	54	V	H	56	W	H	56	W	H	59	W	H	52	L	H	52	L	H	52	L	H
	H2	1	1	1	74	A	H	55	E	H	55	E	H	57	E	H	57	E	H	60	E	H	53	E	H	53	E	H	53	E	H
	H2	1	1	1	75	I	H	56	I	H	56	I	H	58	M	H	58	M	H	61	M	H	54	A	H	54	A	H	54	C	H
	H2	1	1	1	76	V	H	57	A	H	57	A	H	59	A	H	59	A	H	62	T	H	55	L	H	55	L	H	55	A	H
	H2			1	77	T	H	58	R	H	58	R	H	60	D	H	60	D	H	63	D	H	56	D	H	56	D	H	56	G	H
	H2			1	78	A	H	59	K	H	59	K	H	61	F	H	61	F	H	64	Y	H	57	F	H	57	F	H	57	F	H
	H2		1	1	79	V	H	60	L	H	60	L	H	62	L	H	62	L	H	65	L	H	58	F	H	58	F	H	58	L	H
	H2		1	1	80	Q	H	61	M	T	61	M	T	63	L	H	63	L	H	66	V	H	59	K	G	59	K	G	59	K	H
		1	1	1	81	E	H	62	E	T	62	E	T	64	K	T	64	K	T	67	E	H	60	P	G	60	P	G	60	D	T
		1	1	1	82	R	H																								
		1	1	1	83	Y	S	63	F	S	63	F	S	65	K	T	65	K	T	68	Q	T	61	H	G	61	H	G	61	K	T
		1	1	1	84	P		64	D		64	D		66	R	T	66	R	T	69	G	T	62	E		62	E		62	G	T
		1	1	1	85	L		65	I		65	I		67	I		67	I		70	I		63	I		63	I		63	V	
		1	1	1	86	A	S	66	K	S	66	K	S	68	K	S	68	K	S	71	K	S	64	E	S	64	E	S	64	D	S
S3		1	1	1	87	L	E	67	M	E	67	M	E	69	M	E	69	M	E	72	M	E	65	L		65	L	E	65	I	E
S3		1	1	1	88	A	E	68	L	E	68	L	E	70	L	E	70	L	E	73	L	E	66	L	E	66	L	E	66	I	E
S3		1	1	1	89	V	E	69	V	E	69	V	E	71	V	E	71	V	E	74	V	E	67	I	E	67	I	E	67	V	E
S3		1	1	1	90	V	E	70	I	E	70	I	E	72	I	E	72	I	E	75	I	E	68	V	E	68	V	E	68	V	E

Figure 2E

		1	1	1	91	A		71	A		71	A		73	A		73	A		76	A		69	A		69	A		69	A	
		1	1	1	92	C		72	C		72	C		74	C		74	C		77	C	S	70	C		70	C		70	C	
	H3	1	1	1	93	N	H	73	N	H	73	N	H	75	N	H	75	N	H	78	N	H	71	N	H	71	N	H	71	N	H
	H3	1	1	1	94	T	H	74	T	H	74	T	H	76	T	H	76	T	H	79	T	H	72	T	H	72	T	H	72	T	H
	H3	1	1	1	95	A	H	75	A	H	75	A	H	77	A	H	77	A	H	80	A	H	73	A	H	73	A	H	73	A	H
	H3	1	1	1	96	S	H	76	T	H	76	T	H	78	T	H	78	T	H	81	T	H	74	S	H	74	S	H	74	S	H
	H3	1	1	1	97	T	H	77	A	H	77	A	H	79	A	H	79	A	H	82	A	H	75	A	H	75	A	H	75	A	T
	H3	1	1	1	98	V	H	78	V	H	78	V	H	80	V	H	80	V	H	83	V	H	76	L	H	76	L	H	76	Y	T
		1	1	1	99	S	H	79	A	H	79	A	H	81	A	H	81	A	H	84	A	T	77	A	T	77	A	H	77	A	S
	H4	1	1	1	100	L	H	80	L	H	80	L	H	82	L	H	82	L	H	85	L	H	78	L	H	78	L	H	78	L	H
	H4	1	1	1	101	P	H	81	E	H	81	E	H	83	E	H	83	E	H	86	E	H	79	E	H	79	E	H	79	E	H
	H4	1	1	1	102	A	H	82	Y	H	82	Y	H	84	E	H	84	E	H	87	E	H	80	E	H	80	E	H	80	R	H
	H4	1	1	1	103	L	H	83	L	H	83	L	H	85	I	H	85	I	H	88	I	H	81	M	H	81	M	H	81	L	H
	H4	1	1	1	104	R	H	84	E	H	84	E	H	86	K	H	86	K	H	89	K	H	82	Q	H	82	Q	H	82	K	H
	H4	1	1	1	105	E	H	85	K	H	85	K	H	87	A	H	87	A	H	90	A	H	83	K	H	83	K	H	83	K	H
		1	1	1	106	K	H	86	T	H	86	T	H	88	A	H	88	A	H	91	A	H	84	Y	S	84	Y	T	84	E	H
		1	1	1	107	F		87	L		87	L	S	89	L		89	L		92	L		85	S		85	S		85	I	S
		1	1	1	108	D	S	88	S	S	88	S	S	90	P	S	90	P	S	93	S	S	86	K	S	86	K	S	86	N	S
		1	1	1	109	F	S	89	I	S	89	I	S	91	I	S	91	I	S	94	I	S	87	I	S	87	I	S	87	V	S
		1	1	1	110	P		90	S	E	90	S	E	92	P		92	P		95	P		88	P		88	P		88	P	

Figure 2F

S4		1	1	1	111	V	E	91	V	E	91	V	E	93	V	E	93	V	E	96	V	E	89	I	E	89	I	E	89	V	E
S4		1	1	1	112	V	E	92	I	E	92	I	E	94	V	E	94	V	E	97	I	E	90	V	E	90	V	E	90	F	E
		1	1	1	113	G		93	G	E	93	G	E	95	G		95	G		98	G		91	G	E	91	G	E	91	G	E
		1	1	1	114	V		94	V	S	94	V	S	96	V	S	96	V	S	99	V	S	92	V	S	92	V	S	92	V	S
				2	115	V		95	I	H	95	I	H	97	I	H	97	I	S	100	I	S	93	I	S	93	I	S	93	I	H
	H5			2				96	E	H	96	E	H	98	L	H	98	L	H	101	L	H	94	E	H	94	E	H	94	E	H
	H5			2	116	P		97	P	H	97	P	H	99	P	H	99	P	H	102	P	H	95	P	H	95	P	H	95	P	H
	H5	2	2	2	117	A		98	G	H	98	G	H	100	G	H	100	G	H	103	G	H	96	S	H	96	S	H	96	G	H
	H5	2	2	2	118	I	H	99	A	H	99	A	H	101	A	H	101	A	H	104	T	H	97	I	H	97	I	H	97	V	H
	H5	2	2	2	119	K	H	100	R	H	100	R	H	102	R	H	102	R	H	105	R	H	98	L	H	98	L	H	98	K	H
	H5	2	2	2	120	P	H	101	T	H	101	T	H	103	A	H	103	A	H	106	A	H	99	A	H	99	A	H	99	E	H
	H5		2	2	121	A	H	102	A	H	102	A	H	104	A	H	104	A	H	107	A	H	100	I	H	100	I	H	100	A	H
	H5	2	2	2	122	A	H	103	I	H	103	I	H	105	V	H	105	V	H	108	V	H	101	K	H	101	K	H	101	L	H
	H5	2	2	2	123	R	H	104	M	H	104	M	H	106	K	H	106	K	H	109	K	H	102	R	H	102	R	H	102	K	H
	H5	2		2	124	L	H	105	T	H	105	T	H	107	V	H	107	V	H	110	K	H	103	Q	H	103	Q	H	103	K	H
				2	125	T		106	T		106	T		108	T		108	T		111	T		104	V		104	V		104	S	
				2	126	A	S	107	R	S	107	R	S	109	K	S	109	K	S	112	Q	S	105	E		105	E		105	R	S
				2	127	N	S	108	N	S	108	N	S	110	N	S	110	N	S	113	N	S	106	D		106	D		106	N	S
																							107	K	T	107	K	T			
																							108	N	T	108	N	T			

Figure 2G

				2	128	G	S	109	Q	S	109	Q	S	111	N	S	111	N	S	114	K	S	109	A	S	109	A	S	107	K	
		2	2	2	129	I	E	110	N	E	110	N	E	112	K	E	112	K	E	115	Q	E	110	P		110	P		108	K	E
S5		2	2	2	130	V	E	111	V	E	111	V	E	113	I	E	113	I	E	116	V	E	111	I	E	111	I	E	109	I	E
S5		2	2	2	131	G	E	112	L	E	112	L	E	114	G	E	114	G	E	117	G	E	112	L	E	112	L	E	110	G	E
S5		2	2	2	132	L	E	113	V	E	113	V	E	115	V	E	115	V	E	118	I	E	113	V	E	113	V	E	111	V	E
S5		2	2	2	133	L	E	114	L	E	114	L	E	116	I	E	116	I	E	119	I	E	114	L	E	114	L	E	112	I	E
S5		2	2	2	134	A	E	115	G	E	115	G	E	117	G	E	117	G	E	120	G	E	115	G	E	115	G	E	113	G	E
		2	2	2	135	T		116	T		116	T		118	T		118	T		121	T		116	T		116	T		114	T	
	H6	2	2	2	136	R	T	117	E	H	117	E	H	119	L	H	119	L	H	122	I	H	117	K	H	117	K	H	115	P	H
	H6	2	2	2	137	G	T	118	G	H	118	G	H	120	G	H	120	G	H	123	G	H	118	A	H	118	A	H	116	A	H
	H6	2	2	2	138	T	G	119	T	H	119	T	H	121	T	H	121	T	H	124	T	H	119	T	H	119	T	H	117	T	H
	H6	2	2	2	139	V	G	120	I	H	120	I	H	122	I	H	122	I	H	125	V	H	120	I	H	120	I	H	118	V	H
	H6	2	2	2	140	K	G	121	K	H	121	K	H	123	K	H	123	K	H	126	K	H	121	Q	H	121	Q	H	119	K	H
	H6	2	2	2	141	R		122	S	H	122	S	H	124	S	H	124	S	T	127	S	H	122	S	T	122	S	H	120	S	H
			2	2	142	S	H	123	E	T	123	E	T	125	A	T	125	A	T	128	Q	T	123	N	T	123	N	T	121	G	
	H7		2	2	143	Y	H	124	A	H	124	A	H	126	S	H	126	S	H	129	A	H	124	A	H	124	A	H	122	A	H
	H7		2	2	144	T	H	125	Y	H	125	Y	H	127	Y	H	127	Y	H	130	Y	H	125	Y	H	125	Y	H	123	Y	H
	H7		2	2	145	H	H	126	R	H	126	R	H	128	D	H	128	E	H	131	E	H	126	D	H	126	D	H	124	Q	H
	H7		2	2	146	E	H	127	T	H	127	T	H	129	I	H	129	I	H	132	K	H	127	N	H	127	N	H	125	R	H
	H7		2	2	147	L	H	128	H	H	128	H	H	130	A	H	130	A	H	133	A	H	128	A	H	128	A	H	126	K	H

Figure 2H

	H7		2	2	148	I	H	129	I	H	129	I	H	131	I	H	131	I	H	134	L	H	129	L	H	129	L	H	127	L	H
	H7			2	149	A	H	130	K	H	130	K	H	132	K	H	132	K	H	135	K	H	130	K	H	130	K	H	128	E	H
	H7			2	150	R	H	131	R	H	131	R	H	133	S	H	133	S	T	136	E	H	131	Q	H	131	Q	H	129	E	T
				2	151	F	S	132	I	H	132	I	H	134	K	H	134	K	T	137	K	H	132	Q	T	132	Q	T	130	G	T
				2	152	A		133	N		133	N		135	A		135	A		138	V		133	G	T	133	G	T			
				2	153	N	T	134	P	T	134	P	T	136	P	T	136	P	T	139	P	T									
				2	154	E	T	135	H	T	135	H	T	137	A	T	137	A	T	140	E	T	134	Y		134	Y		131	G	S
				2	155	C	S	136	V		136	V		138	I	S	138	I		141	L		135	L		135	L		132	A	
		2	2	2	156	Q	E	137	E	E	137	E	E	139	E	E	139	E	E	142	T	E	136	N		136	N		133	D	E
S6		2	2	2	157	I	E	138	V	E	138	V	E	140	V	E	140	V	E	143	V	E	137	I	E	137	I	E	134	V	E
S6		2	2	2	158	E	E	139	H	E	139	H	E	141	T	E	141	T	E	144	T	E	138	S	E	138	S	E	135	F	E
S6		2	2	2	159	M	E	140	G	E	140	G	E	142	S	E	142	S	E	145	S	E	139	H	E	139	H	E	136	A	E
S6		2	2	2	160	L	E	141	V	E	141	V	E	143	L	E	143	L	E	146	L	E	140	L	E	140	L	E	137	K	E
S6		2	2	2	161	G	E	142	A	E	142	A	E	144	A	E	144	A	E	147	A	E	141	A	E	141	A	E	138	A	E
				2	162	S		143	C		143	C		145	C		145	C		148	C		142	T		142	T		139	C	
				2	163	A	H	144	P	T	144	P	T	146	P	T	146	P	T	149	P	T	143	S	T	143	S	T	140	P	
					164	E	H	145	G	T	145	G	T	147	K	T	147	K	T	150	K	T	144	L	T	144	L	T	141	L	
	H8			2	165	M	H	146	F	H	146	F	H	148	F	H	148	F	H	151	F	H	145	F	H	145	F	H	142	F	
	H8			2	166	V	H	147	V	H	147	V	H	149	V	H	149	V	H	152	V	H	146	V	H	146	V	H	143	A	T
	H8			2	167	E	H	148	P	H	148	P	H	150	P	H	150	P	H	153	S	H	147	P	H	147	P	H	144	P	T

Figure 2I

	H8			2	168	L	H	149	L	H	149	L	H	151	I	H	151	I	H	154	V	H	148	L	H	148	L	H	145	L	T
	H8			2	169	A	H	150	V	H	150	V	H	152	V	H	152	V	H	155	V	H	149	I	H	149	I	H	146	A	S
	H8			2	170	E	H	151	E	H	151	E	H	153	E	H	153	E	H	156	E	H	150	E	H	150	E	H	147	E	
				2	171	A	H	152	Q	T	152	Q	H	154	S	T	154	S	T	157	S	T	151	E	T	151	E	T	148	E	G
				2	172	K	H	153	M	T	153	M		155	N	T	155	N	T	158	N	T	152	S	T	152	S	T	149	G	G
				2	173	L	H	154	R		154	R	S	156	Q		156	Q		159	E		153	I		153	I		150	L	G
				2	174	H	H	155	Y	T	155	Y	S	157	Y	T	157	Y	S	160	Y	T	154	L		154	L		151	L	G
				2	175	G	T	156	S	T	156	S		158	R	T	158	R	S	161	H	T	155	E	S	155	E	S	152	E	S
				2	176	E		157	D		157	D	H	159	S	S	159	S	S	162	S	S	156	G	S	156	G	H	153	G	G
								158	P	H	158	P																			
				2	177	D		159	T	H	159	T	H	160	S	H	160	S	H	163	S	H	157	E	H	157	E	H	154	E	G
				2	178	V		160	V	H	160	I	H	161	V	H	161	V	H	164	V	H	158	L	H	158	L	H	155	I	G
	H9			2	179	S		161	I	H	161	I	H	162	A	H	162	A	H	165	A	H	159	L	H	159	L	H	156	T	H
	H9	2	2	2	180	L	H	162	S	H	162	S	H	163	K	H	163	K	H	166	K	H	160	E	H	160	E	H	157	R	H
	H9	2	2	2	181	D	H	163	I	H	163	I	H	164	K	H	164	K	H	167	K	H	161	T	H	161	T	H	158	K	H
	H9	2	2	2	182	A	H	164	V	H	164	V	H	165	I	H	165	I	H	168	I	H	162	C	H	162	C	H	159	V	H
	H9	2	2	2	183	L	H	165	I	H	165	I	H	166	V	H	166	V	H	169	V	H	163	M	H	163	M	H	160	V	H
	H9	2	2	2	184	K	H	166	H	H	166	H	H	167	A	H	167	A	H	170	A	H	164	H	H	164	H	H	161	E	H
	H9	2		2	185	R	H	167	Q	H	167	Q	H	168	E	H	168	E	H	171	E	H	165	Y	H	165	Y	H	162	H	H
	H9	2		2	186	I	H	168	T	H	168	T	H	169	T	H	169	T	H	172	T	H	166	Y	H	166	Y	H	163	Y	H

Figure 2J

		2		2	187	L	T	169	L	H	169	L	H	170	L	H	170	L	T	173	L	H	167	F	H	167	F	H	164	L	S
		2		2	188	R	H	170	K	G	170	K	G	171	Q	G	171	Q	T	174	A	G	168	T	T	168	T	T	165	K	T
				2	189	P	H	171	R	G	171	R	G	172	A	G	172	A	G	175	P	G	169	P	T	169	P	T	166	E	T
				2	190	W	H	172	W	G	172	W	G	173	L	G	173	L	G	176	L	G	170	L		170	L		167	F	T
				2	191	L	H	173	R	T	173	R	T	174	Q	T	174	Q	G	177	T	G	171	E	S	171	E	S	168	K	T
					192	R	T	174	N	T	174	N	T	175	L	T	175	L	G	178	T	G	172	I	S	172	I	S	169	G	T
				2	193	M		175	S		175	S		176	K	S	176	K	T	179	K	S									
				2	194	K	S																								
					195	E	S																								
					196	P		176	E	S	176	E	S	177	G		177	G		180	K		173	L		173	L		170	K	T
		2	2	2	197	P		177	S		177	S		178	L		178	L		181	I		174	P		174	P		171	I	
		2	2	2	198	D	S	178	D	S	178	D	S	179	D	S	179	D	S	182	D		175	E	S	175	E	S	172	D	S
S7		2	2	2	199	T	E	179	T	E	179	T	E	180	T	E	180	T	E	183	T	E	176	V	E	176	V	E	173	T	E
S7		2	2	2	200	V	E	180	V	E	180	V	E	181	L	E	181	L	E	184	L	E	177	I	E	177	I	E	174	L	E
S7		2	2	2	201	V	E	181	I	E	181	I	E	182	I	E	182	I	E	185	I	E	178	I	E	178	I	E	175	I	E
S7		2	2	2	202	L	E	182	L	E	182	L	E	183	L	E	183	L	E	186	L	E	179	L	E	179	L	E	176	L	E
		2	2	2	203	G		183	G	E	183	G	E	184	G		184	G		187	G		180	G	E	180	G		177	G	
				2	204	C	S	184	C	S	184	C	S	185	C	S	185	C	S	188	C	S	181	C	S	181	C	S	178	C	
				2	205	T	T	185	T	S	185	T	T	186	T	T	186	T	T	189	T	T	182	T	S	182	T	T	179	T	
				2	206	H	T	186	H	S	186	H	T	187	H	T	187	H	T	190	H	T	183	H	S	183	H	T	180	H	

Figure 2K

				2	207	F	G	187	Y	G	187	Y	G	188	Y	G	188	Y	G	191	Y	G	184	F	G	184	F	G	181	Y	T
				2	208	P	G	188	P	G	188	P	G	189	P	G	189	P	G	192	P	G	185	P	G	185	P	G	182	P	T
				2	209	L	G	189	L	G	189	L	G	190	L	G	190	L	G	193	L	G	186	L	G	186	L	G	183	L	
				2	210	L	G	190	L	G	190	L	G	191	L	G	191	L	G	194	L	G	187	I	G	187	I	G	184	L	
	H10	2	2	2	211	Q	H	191	Y	H	191	Y	H	192	R	H	192	R	H	195	R	H	188	A	H	188	A	H	185	K	H
	H10	2	2	2	212	E	H	192	K	H	192	K	H	193	P	H	193	P	H	196	P	H	189	Q	H	189	Q	H	186	K	H
	H10	2	2	2	213	E	H	193	P	H	193	P	H	194	V	H	194	V	H	197	I	H	190	K	H	190	K	H	187	E	H
	H10	2	2	2	214	L	H	194	I	H	194	I	H	195	I	H	195	I	H	198	I	H	191	I	H	191	I	H	188	I	H
	H10	2	2	2	215	L	H	195	Y	H	195	Y	H	196	Q	H	196	Q	H	199	Q	H	192	E	H	192	E	H	189	K	H
	H10	2	2	2	216	Q	H	196	D	H	196	D	H	197	N	H	197	N	H	200	N	H	193	G	H	193	G	H	190	K	H
	H10	2	2	2	217	V	H	197	Y	H	197	Y	H	198	V	H	198	V	H	201	V	H	194	Y	H	194	Y	H	191	F	H
		2	2	2	218	L	S	198	F	T	198	F	T	199	M	H	199	M	H	202	M	H	195	F	H	195	F	H	192	L	S
			2	2	219	P		199	G	T	199	G	T	200	G		200	G		203	G		196	M	H	196	M	H	193	G	
																						197	G	H	197	G	H				
																						198	H	H	198	H	H				
																						199	F	T	199	F	T				
																						200	A	T	200	A	T				
																						201	L		201	L					
																						202	P	S	202	P	S				
				2	220	E	T	200	G	T	200	G	T	201	S	T	201	S	T	204	E	T	203	T	S	203	T	S			

Figure 2L

				2	221	G	T	201	K		201	K		202	H	T	202	H	T	205	N	T	204	P		204	P		194	D	S
		2	2	2	222	T		202	K	S	202	K		203	V		203	V		206	V	S	205	P		205	P		195	A	
S8		2	2	2	223	R	E	203	T	E	203	T	E	204	T	E	204	T	E	207	Q	E	206	L	E	206	L	E	196	E	E
S8		2	2	2	224	L	E	204	V	E	204	V	E	205	L	E	205	L	E	208	L	E	207	L	E	207	L	E	197	V	E
S8		2	2	2	225	V	E	205	I	E	205	I	E	206	I	E	206	I	E	209	I	E	208	I	E	208	I	E	198	V	E
			2	2	226	D		206	S	E	206	S	E	207	D	E	207	D	E	210	D	E	209	H	E	209	H	E	199	D	
					227	S	S	207	S	H	207	S	H	208	S	H	208	S	H	211	S	H	210	S	H	210	S	H	200	S	H
	H11	1		1	228	G	H	208	G	H	208	G	H	209	G	H	209	G	H	212	G	H	211	G	H	211	G	H	201	S	H
	H11	1		1	229	A	H	209	L	H	209	L	H	210	A	H	210	A	H	213	A	H	212	D	H	212	D	H	202	E	H
	H11	1	1	1	230	A	H	210	E	H	210	E	H	211	E	H	211	E	H	214	E	H	213	A	H	213	A	H	203	A	H
	H11	1	1	1	231	I	H	211	T	H	211	T	H	212	T	H	212	T	H	215	T	H	214	I	H	214	I	H	204	L	H
	H11	1	1	1	232	A	H	212	A	H	212	A	H	213	V	H	213	V	H	216	V	H	215	V	H	215	V	H	205	S	H
	H11	1	1	1	233	R	H	213	R	H	213	R	H	214	G	H	214	G	H	217	G	H	216	E	H	216	E	H	206	L	H
	H11	1	1	1	234	R	H	214	E	H	214	E	H	215	E	H	215	E	H	218	E	H	217	Y	H	217	Y	H	207	S	T
	H11	1	1	1	235	T	H	215	V	H	215	V	H	216	V	H	216	V	H	219	V	H	218	L	H	218	L	H	208	L	T
	H11	1	1	1	236	A	H	216	S	H	216	S	H	217	S	H	217	S	H	220	S	H	219	Q	H	219	Q	H	209	H	T
	H11	1	1	1	237	W	H	217	A	H	217	A	H	218	M	H	218	M	H	221	M	H	220	Q	H	220	Q	H	210	N	T
	H11			1	238	L	H	218	L	H	218	L	H	219	L	H	219	L	H	222	L	H	221	K	T	221	K	H	211	F	T
				1	239	L	H	219	L	H	219	L	H	220	L	H	220	L	H	223	L	H	222	Y	T	222	Y	T	212	I	
				1	240	E	H	220	T	H	220	T	H	221	D	H	221	D	H	224	D	H	223	A	T	223	A	T	213	K	

Figure 2M

				1	241	H	H	221	F	H	221	F	H	222	Y	H	222	Y	H	225	Y	H	224	L		224	L		214	D	
				1	242	E	T	222	S	T	222	S	T	223	F	T	223	F	H	226	F	T	225	K		225	K		215	D	
				1	243	A		223	N	T	223	N	T	224	D	T	224	D	T	227	N	T	226	N	T	226	N	S	216	G	S
				1	244	P		224	E		224	E		225	I		225	I		228	L		227	N	T	227	N		217	S	
				1	245	D	S	225	H		225	H		226	A		226	A		229	S		228	A	S	228	A	S	218	S	
				1	246	A		226	A		226	A		227	H		227	H		230	N		229	C		229	C		219	S	
				1	247	K	E	227	S		227	S		228	T		228	T		231	S		230	T	S	230	T	S			
					248	S	E	228	Y		228	Y		229	P	S	229	P	S	232	P	T	231	F	S	231	F	S			
					249	A		229	T		229	T	S	230	E	S	230	E	S	233	Q	T	232	P		232	P				
					250	D	S	230	E	S	230	E	S	231	A		231	A	S	234	N		233	K	E	233	K	E			
					251	A		231	H	S	231	H		232	P		232	P		235	G										
								232	P		232	P		233	T	S	233	T		236	R										
								233	D		233	D		234	Q	S	234	Q		237	T										
														235	P		235	P		238	L										
		1	1	1	252	N		234	H		234	H		236	H		236	H		239	C	E	234	V	E	234	V	E			
S9		1	1	1	253	I	E	235	R	E	235	R	E	237	E	E	237	E	E	240	Q	E	235	E	E	235	E	E			
S9		1	1	1	254	A	E	236	F	E	236	F	E	238	F	E	238	F	E	241	F	E	236	F	E	236	F	E			
S9		1	1	1	255	F	E	237	F	E	237	F	E	239	Y	E	239	Y	E	242	Y	E	237	H	E	237	H	E			
S9		1	1	1	256	C	E	238	A	E	238	A	E	240	T	E	240	T	E	243	T	E	238	A	E	238	A	E			
		1	1	1	257	M	S	239	T	S	239	T	S	241	T	S	241	T	S	244	T	S	239	S	S	239	S	S			

Figure 2N

			1	1	258	A	S	240	G	S	240	G	S	242	G	S	242	G	S	245	G	S	240	G	S	240	G	S			
				1	259	M		241	D		241	D		243	S		243	S		246	S		241	D		241	D				
				1	260	T		242	T		242	T		244	A	H	244	A	H	247	A	H	242	V	H	242	V	H			
	H12			1	261	P	H	243	T	H	243	T	H	245	K	H	245	K	H	248	K	H	243	I	H	243	I	H			
	H12			1	262	G	H	244	H	H	244	H	H	246	M	H	246	M	H	249	L	H	244	W	H	244	W	H			
	H12		1	1	263	A	H	245	I	H	245	I	H	247	F	H	247	F	H	250	F	H	245	L	H	245	L	H			
	H12		1	1	264	E	H	246	T	H	246	T	H	248	E	H	248	E	H	251	E	H	246	E	H	246	E	H			
	H12		1	1	265	Q	T	247	N	H	247	N	H	249	E	H	249	E	H	252	E	H	247	R	H	247	R	H			
	H12		1	1	266	L	T	248	I	H	248	I	H	250	I	H	250	I	H	253	I	H	248	Q	H	248	Q	H			
	H12		1	1	267	L	H	249	I	H	249	I	H	251	A	H	251	A	H	254	A	H	249	A	H	249	A	H			
	H12		1	1	268	P	H	250	K	H	250	K	H	252	S	H	252	S	H	255	E	H	250	K	H	250	K	H			
	H12		1	1	269	V	H	251	E	H	251	E	H	253	S	H	253	S	H	256	D	H	251	E	H	251	E	H			
	H12		1	1	270	L	H	252	W	H	252	W	H	254	W	H	254	W	H	257	W	H	252	W	H	252	W	H			
	H12		1	1	271	Q	H	253	L	H	253	L	H	255	L	H	255	L	H	258	L	H	253	L	H	253	L	H			
				1	272	R	H	254	N		254	N		256	G	T	256	G		259	G		254	K		254	K				
				1	273	Y	T	255	L		255	L		257	I		257	I		260	I	S	255	L		255	L				
				1	274	G	T	256	S		256	S		258	E	T	258	E	S	261	G	S									
				1	275	F		-						259	N	T	259	N	S	262	H										
				1	276	E		257	V		257	V		260	L		260	L		263	L										
S10				1	277	T	E	258	N		258	N	E	261	K		261	K		264	N	E							Pylori off		

Figure 20

S10				**1**	**278**	**L**	**E**	**259**	**V**		**259**	**V**	**E**	**262**	**A**		**262**	**A**	**E**	**265**	**V**	**E**								
S10				**1**	**279**	**E**	**E**	**260**	**E**	**E**	**260**	**E**		**263**	**Q**	**E**	**263**	**Q**	**E**	**266**	**E**	**E**								
				1	280	K	E	261	R	E	261	R		264	Q	E	264	Q	E	267	H	E								
				1	281	L		262	I		262	I		265	I		265	I		268	I									
				1	282	A		263	S		263	S		266	H		266	H		269	E									
				1	283	V		264	V		264	V		267	L		267	L		270	L									
					284	L		265	N		265	N		268	G		268	G		271	G									
					285	G														272	G									
																				273	G									

1 = Domain one
2 = Domain two

E = Strand
H = Hinge
S&T = Loops and Turns

Code for core elements:
Orange = all Muri's
Magenta= all - E coli
Green= Only gram+

Figure 3

Domain/ Species	Ligand	cα-cα distance active site cysteines	cα-cα distance between Asp7* and Gly115*	S-S distance for active site cysteines	Dyndom angle	Angle as defined by the angle between residue Val215* and ca positions of Asp7* and Gly115*
Disulfide	Empty	4.7 Å		2.0 Å		Not calculated
E. faecalis	D-Glu	7.2 Å	14.7 Å	7.5 Å	11°	50.2°
E. faecalis	L-Glu	6.8 Å	14.1 Å	6.9 Å	0°	45.9°
E. coli	L-Glu	7.0 Å	14.9 Å	7.6 Å		45.5°
H. pylori	D-Glu	7.0 Å	14.7 Å	7.5 Å		45.2°
S. aureus	D-Glu	7.0 Å	14.8 Å	7.3 Å		45.5°
E. faecium	Citrate	7.5 Å	15.6 Å	9.1 Å		53.3°
E. faecium	Tartrate	8.7 Å	15.8 Å	10.1 Å		53.7°
E. faecium	Phosphate	8.2 Å	16.0 Å	10.4 Å	18 (model)	54.2°
A. pyrophilus	empty	9.4 Å	15.5 Å	11.3 Å		51.6°

**H. pylori* residue numbers

Figure 4A

```
REMARK Created by MOLEMAN V. 991230/7.3 at Tue Dec 10 19:34:52 2002 for kemitl
REMARK MoleMan PDB file
REMARK Created by MOLEMAN V. 961218/7.2.5 at Tue Mar 28 15:09:11 2000 for kemitl
REMARK MoleMan PDB file
REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 1.86 A
REMARK starting r= 0.2208 free_r= 0.2457
REMARK final   r= 0.2055 free_r= 0.2376
REMARK B rmsd for bonded mainchain atoms=  1.483  target= 1.5
REMARK B rmsd for bonded sidechain atoms=  2.506  target= 2.0
REMARK B rmsd for angle mainchain atoms=  2.042  target= 2.0
REMARK B rmsd for angle sidechain atoms=  3.617  target= 2.5
REMARK wa= 1.64705
REMARK rweight=6.377507E-02
REMARK target= mlf  steps= 50
REMARK sg= P2(1)2(1)2(1) a= 61.41 b= 76.31 c= 108.92 alpha= 90 beta= 90 gamma= 90
REMARK parameter file 1  : MSI_CNX_TOPPAR:protein_rep.param
REMARK parameter file 2  : MSI_CNX_TOPPAR:water_rep.param
REMARK parameter file 3  : inh.par
REMARK parameter file 4  : gld.par
REMARK molecular structure file: generate_easy.psf
REMARK input coordinates: bgroup.pdb
REMARK reflection file= muri_1.8.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.86
REMARK initial B-factor correction applied to fobs :
REMARK   B11=   0.497 B22=   1.667 B33=  -2.164
REMARK   B12=   0.000 B13=   0.000 B23=   0.000
REMARK B-factor correction applied to coordinate array B:    1.176
REMARK bulk solvent: (Mask) density level= 0.365438 e/A^3, B-factor= 33.2255 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range:    43743 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):   3410 (   7.8 % )
REMARK number of reflections rejected:                          0 (   0.0 % )
REMARK total number of reflections used:                    40333 (  92.2 % )
REMARK number of reflections in working set:                38313 (  87.6 % )
REMARK number of reflections in test set:                   2020 (   4.6 % )
REMARK FILENAME="bindividual.pdb"
REMARK DATE:Mar-24-2000  16:16:02      created by user: kemitl
REMARK Written by CNX VERSION:2000
CRYST1  61.410  76.310 108.920  90.00  90.00  90.00 P212121      1
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.016284  0.000000  0.000000        0.00000
SCALE2      0.000000  0.013104  0.000000        0.00000
SCALE3      0.000000  0.000000  0.009181        0.00000
ATOM      1  CB  MET A   1      30.124  48.907  56.585  1.00 22.42      A    C
ATOM      2  CG  MET A   1      30.702  50.302  56.333  1.00 25.22      A    C
ATOM      3  SD  MET A   1      31.489  51.055  57.785  1.00 28.98      A    S
ATOM      4  CE  MET A   1      32.951  49.983  58.010  1.00 26.14      A    C
ATOM      5  C   MET A   1      27.890  49.690  57.412  1.00 19.35      A    C
ATOM      6  O   MET A   1      27.114  49.386  56.503  1.00 20.53      A    O
ATOM      7  N   MET A   1      28.658  47.421  57.925  1.00 18.28      A    N
ATOM      8  CA  MET A   1      29.106  48.829  57.729  1.00 20.61      A    C
ATOM      9  N   LYS A   2      27.729  50.760  58.178  1.00 18.84      A    N
ATOM     10  CA  LYS A   2      26.605  51.666  58.005  1.00 19.29      A    C
```

Figure 4B

```
ATOM   11  CB  LYS A   2      25.834  51.769  59.316  1.00 18.82      A   C
ATOM   12  CG  LYS A   2      24.636  52.702  59.295  1.00 20.09      A   C
ATOM   13  CD  LYS A   2      24.005  52.752  60.674  1.00 22.85      A   C
ATOM   14  CE  LYS A   2      22.697  53.523  60.676  1.00 22.98      A   C
ATOM   15  NZ  LYS A   2      22.078  53.501  62.033  1.00 22.51      A   N
ATOM   16  C   LYS A   2      27.131  53.031  57.588  1.00 17.25      A   C
ATOM   17  O   LYS A   2      27.980  53.616  58.265  1.00 16.44      A   O
ATOM   18  N   ILE A   3      26.630  53.533  56.464  1.00 17.70      A   N
ATOM   19  CA  ILE A   3      27.075  54.824  55.968  1.00 14.65      A   C
ATOM   20  CB  ILE A   3      28.001  54.647  54.738  1.00 16.82      A   C
ATOM   21  CG2 ILE A   3      29.214  53.807  55.121  1.00 17.12      A   C
ATOM   22  CG1 ILE A   3      27.252  53.971  53.593  1.00 17.27      A   C
ATOM   23  CD1 ILE A   3      26.697  54.929  52.583  1.00 20.09      A   C
ATOM   24  C   ILE A   3      25.925  55.758  55.617  1.00 14.64      A   C
ATOM   25  O   ILE A   3      24.752  55.377  55.639  1.00 14.39      A   O
ATOM   26  N   GLY A   4      26.269  57.001  55.322  1.00 13.89      A   N
ATOM   27  CA  GLY A   4      25.244  57.956  54.961  1.00 14.96      A   C
ATOM   28  C   GLY A   4      25.500  58.490  53.569  1.00 13.26      A   C
ATOM   29  O   GLY A   4      26.634  58.453  53.081  1.00 11.89      A   O
ATOM   30  N   VAL A   5      24.439  58.954  52.917  1.00 11.22      A   N
ATOM   31  CA  VAL A   5      24.549  59.541  51.592  1.00 10.79      A   C
ATOM   32  CB  VAL A   5      23.964  58.625  50.500  1.00 14.07      A   C
ATOM   33  CG1 VAL A   5      23.918  59.363  49.169  1.00 12.77      A   C
ATOM   34  CG2 VAL A   5      24.828  57.385  50.352  1.00 12.02      A   C
ATOM   35  C   VAL A   5      23.771  60.848  51.643  1.00 11.63      A   C
ATOM   36  O   VAL A   5      22.596  60.872  52.020  1.00 12.22      A   O
ATOM   37  N   PHE A   6      24.445  61.932  51.287  1.00 11.51      A   N
ATOM   38  CA  PHE A   6      23.848  63.256  51.302  1.00 13.29      A   C
ATOM   39  CB  PHE A   6      24.674  64.182  52.203  1.00 13.43      A   C
ATOM   40  CG  PHE A   6      24.252  65.620  52.143  1.00 14.85      A   C
ATOM   41  CD1 PHE A   6      22.937  65.981  52.418  1.00 16.29      A   C
ATOM   42  CD2 PHE A   6      25.164  66.612  51.800  1.00 15.26      A   C
ATOM   43  CE1 PHE A   6      22.530  67.317  52.350  1.00 17.43      A   C
ATOM   44  CE2 PHE A   6      24.770  67.954  51.728  1.00 17.55      A   C
ATOM   45  CZ  PHE A   6      23.450  68.305  52.003  1.00 18.07      A   C
ATOM   46  C   PHE A   6      23.725  63.887  49.920  1.00 12.87      A   C
ATOM   47  O   PHE A   6      24.641  63.806  49.102  1.00 14.09      A   O
ATOM   48  N   ASP A   7      22.583  64.519  49.674  1.00 11.45      A   N
ATOM   49  CA  ASP A   7      22.331  65.212  48.418  1.00 12.53      A   C
ATOM   50  CB  ASP A   7      21.749  64.263  47.363  1.00 11.52      A   C
ATOM   51  CG  ASP A   7      21.491  64.959  46.035  1.00 10.71      A   C
ATOM   52  OD1 ASP A   7      22.444  65.525  45.457  1.00 12.13      A   O
ATOM   53  OD2 ASP A   7      20.332  64.944  45.571  1.00 11.62      A   O
ATOM   54  C   ASP A   7      21.353  66.350  48.670  1.00 10.34      A   C
ATOM   55  O   ASP A   7      20.714  66.410  49.716  1.00 12.06      A   O
ATOM   56  N   SER A   8      21.245  67.262  47.713  1.00 12.07      A   N
ATOM   57  CA  SER A   8      20.330  68.387  47.856  1.00 12.93      A   C
ATOM   58  CB  SER A   8      20.595  69.417  46.756  1.00 12.10      A   C
ATOM   59  OG  SER A   8      20.364  68.857  45.474  1.00 10.24      A   O
ATOM   60  C   SER A   8      18.874  67.909  47.783  1.00 13.34      A   C
ATOM   61  O   SER A   8      17.957  68.609  48.217  1.00 14.16      A   O
ATOM   62  N   GLY A   9      18.667  66.709  47.250  1.00 13.06      A   N
ATOM   63  CA  GLY A   9      17.319  66.182  47.143  1.00 12.56      A   C
ATOM   64  C   GLY A   9      17.253  64.728  46.721  1.00 13.45      A   C
ATOM   65  O   GLY A   9      17.886  63.861  47.329  1.00 13.56      A   O
ATOM   66  N   VAL A  10      16.484  64.460  45.671  1.00 12.87      A   N
ATOM   67  CA  VAL A  10      16.323  63.104  45.159  1.00 12.62      A   C
ATOM   68  CB  VAL A  10      14.916  62.935  44.552  1.00 12.47      A   C
```

Figure 4C

```
ATOM   69 CG1 VAL A 10    14.715 63.955 43.453 1.00 11.29    A  C
ATOM   70 CG2 VAL A 10    14.720 61.521 44.031 1.00 12.71    A  C
ATOM   71 C  VAL A 10    17.372 62.785 44.095 1.00 12.55    A  C
ATOM   72 O  VAL A 10    17.586 61.624 43.749 1.00 11.19    A  O
ATOM   73 N  GLY A 11    18.020 63.823 43.575 1.00 12.78    A  N
ATOM   74 CA GLY A 11    19.032 63.623 42.548 1.00 10.57    A  C
ATOM   75 C  GLY A 11    20.039 62.536 42.884 1.00 12.63    A  C
ATOM   76 O  GLY A 11    20.376 61.696 42.035 1.00 12.33    A  O
ATOM   77 N  GLY A 12    20.514 62.560 44.126 1.00 12.27    A  N
ATOM   78 CA GLY A 12    21.488 61.589 44.597 1.00 13.34    A  C
ATOM   79 C  GLY A 12    21.125 60.142 44.331 1.00 12.55    A  C
ATOM   80 O  GLY A 12    21.963 59.252 44.496 1.00 12.07    A  O
ATOM   81 N  PHE A 13    19.877 59.894 43.938 1.00 11.81    A  N
ATOM   82 CA PHE A 13    19.447 58.534 43.619 1.00 12.39    A  C
ATOM   83 CB PHE A 13    18.009 58.515 43.081 1.00 13.67    A  C
ATOM   84 CG PHE A 13    16.947 58.401 44.148 1.00 13.33    A  C
ATOM   85 CD1 PHE A 13    15.671 57.955 43.816 1.00 14.75    A  C
ATOM   86 CD2 PHE A 13    17.215 58.740 45.470 1.00 13.91    A  C
ATOM   87 CE1 PHE A 13    14.667 57.846 44.790 1.00 18.10    A  C
ATOM   88 CE2 PHE A 13    16.221 58.635 46.454 1.00 15.28    A  C
ATOM   89 CZ PHE A 13    14.943 58.186 46.112 1.00 13.91    A  C
ATOM   90 C  PHE A 13    20.361 57.940 42.547 1.00 13.92    A  C
ATOM   91 O  PHE A 13    20.630 56.737 42.551 1.00 12.12    A  O
ATOM   92 N  SER A 14    20.827 58.781 41.625 1.00 13.26    A  N
ATOM   93 CA SER A 14    21.690 58.304 40.547 1.00 13.42    A  C
ATOM   94 CB SER A 14    21.967 59.423 39.525 1.00 13.96    A  C
ATOM   95 OG SER A 14    22.695 60.504 40.071 1.00 12.20    A  O
ATOM   96 C  SER A 14    22.992 57.730 41.092 1.00 13.28    A  C
ATOM   97 O  SER A 14    23.559 56.805 40.509 1.00 14.54    A  O
ATOM   98 N  VAL A 15    23.458 58.270 42.214 1.00 10.88    A  N
ATOM   99 CA VAL A 15    24.674 57.777 42.846 1.00 11.83    A  C
ATOM  100 CB VAL A 15    25.338 58.859 43.730 1.00 11.43    A  C
ATOM  101 CG1 VAL A 15    26.452 58.243 44.580 1.00 10.44    A  C
ATOM  102 CG2 VAL A 15    25.909 59.960 42.849 1.00 11.65    A  C
ATOM  103 C  VAL A 15    24.333 56.566 43.709 1.00 13.82    A  C
ATOM  104 O  VAL A 15    25.068 55.579 43.727 1.00 13.72    A  O
ATOM  105 N  LEU A 16    23.199 56.635 44.400 1.00 13.39    A  N
ATOM  106 CA LEU A 16    22.767 55.546 45.264 1.00 14.00    A  C
ATOM  107 CB LEU A 16    21.479 55.937 45.993 1.00 11.47    A  C
ATOM  108 CG LEU A 16    20.947 54.898 46.991 1.00 14.59    A  C
ATOM  109 CD1 LEU A 16    22.049 54.511 47.980 1.00 13.56    A  C
ATOM  110 CD2 LEU A 16    19.743 55.477 47.733 1.00 10.24    A  C
ATOM  111 C  LEU A 16    22.562 54.246 44.486 1.00 14.34    A  C
ATOM  112 O  LEU A 16    22.879 53.162 44.980 1.00 13.30    A  O
ATOM  113 N  LYS A 17    22.044 54.356 43.267 1.00 14.05    A  N
ATOM  114 CA LYS A 17    21.822 53.176 42.438 1.00 16.52    A  C
ATOM  115 CB LYS A 17    21.229 53.584 41.087 1.00 16.99    A  C
ATOM  116 CG LYS A 17    21.051 52.424 40.114 1.00 21.73    A  C
ATOM  117 CD LYS A 17    20.461 52.893 38.802 1.00 24.05    A  C
ATOM  118 CE LYS A 17    20.298 51.729 37.833 1.00 27.52    A  C
ATOM  119 NZ LYS A 17    19.805 52.178 36.505 1.00 24.97    A  N
ATOM  120 C  LYS A 17    23.136 52.423 42.220 1.00 17.90    A  C
ATOM  121 O  LYS A 17    23.194 51.193 42.319 1.00 16.07    A  O
ATOM  122 N  SER A 18    24.193 53.171 41.931 1.00 16.04    A  N
ATOM  123 CA SER A 18    25.508 52.582 41.691 1.00 17.22    A  C
ATOM  124 CB SER A 18    26.494 53.663 41.248 1.00 16.33    A  C
ATOM  125 OG SER A 18    26.080 54.255 40.034 1.00 15.13    A  O
ATOM  126 C  SER A 18    26.033 51.900 42.944 1.00 16.33    A  C
```

Figure 4D

```
ATOM   127  O   SER A  18      26.579  50.795  42.885  1.00 14.32      A   O
ATOM   128  N   LEU A  19      25.863  52.577  44.075  1.00 13.38      A   N
ATOM   129  CA  LEU A  19      26.301  52.072  45.367  1.00 14.03      A   C
ATOM   130  CB  LEU A  19      26.009  53.102  46.456  1.00 11.70      A   C
ATOM   131  CG  LEU A  19      26.748  54.435  46.350  1.00 12.66      A   C
ATOM   132  CD1 LEU A  19      26.284  55.365  47.471  1.00 13.24      A   C
ATOM   133  CD2 LEU A  19      28.248  54.185  46.442  1.00 11.34      A   C
ATOM   134  C   LEU A  19      25.605  50.771  45.720  1.00 15.80      A   C
ATOM   135  O   LEU A  19      26.240  49.831  46.195  1.00 14.57      A   O
ATOM   136  N   LEU A  20      24.294  50.727  45.496  1.00 15.82      A   N
ATOM   137  CA  LEU A  20      23.510  49.540  45.793  1.00 18.19      A   C
ATOM   138  CB  LEU A  20      22.026  49.807  45.515  1.00 16.40      A   C
ATOM   139  CG  LEU A  20      21.346  50.798  46.473  1.00 16.62      A   C
ATOM   140  CD1 LEU A  20      19.949  51.156  45.974  1.00 16.53      A   C
ATOM   141  CD2 LEU A  20      21.279  50.176  47.867  1.00 16.65      A   C
ATOM   142  C   LEU A  20      23.983  48.330  44.988  1.00 20.92      A   C
ATOM   143  O   LEU A  20      24.179  47.247  45.538  1.00 20.94      A   O
ATOM   144  N   LYS A  21      24.169  48.511  43.687  1.00 20.60      A   N
ATOM   145  CA  LYS A  21      24.612  47.406  42.847  1.00 22.68      A   C
ATOM   146  CB  LYS A  21      24.656  47.840  41.380  1.00 21.65      A   C
ATOM   147  CG  LYS A  21      24.973  46.699  40.426  1.00 26.15      A   C
ATOM   148  CD  LYS A  21      25.083  47.169  38.988  1.00 29.67      A   C
ATOM   149  CE  LYS A  21      25.506  46.017  38.078  1.00 34.31      A   C
ATOM   150  NZ  LYS A  21      25.776  46.469  36.684  1.00 32.80      A   N
ATOM   151  C   LYS A  21      25.978  46.863  43.263  1.00 21.58      A   C
ATOM   152  O   LYS A  21      26.214  45.654  43.208  1.00 23.12      A   O
ATOM   153  N   ALA A  22      26.868  47.753  43.692  1.00 19.68      A   N
ATOM   154  CA  ALA A  22      28.216  47.360  44.093  1.00 19.96      A   C
ATOM   155  CB  ALA A  22      29.131  48.585  44.080  1.00 14.81      A   C
ATOM   156  C   ALA A  22      28.317  46.635  45.446  1.00 20.35      A   C
ATOM   157  O   ALA A  22      29.402  46.199  45.839  1.00 21.92      A   O
ATOM   158  N   ARG A  23      27.198  46.509  46.154  1.00 20.50      A   N
ATOM   159  CA  ARG A  23      27.187  45.821  47.444  1.00 21.19      A   C
ATOM   160  CB  ARG A  23      27.205  44.307  47.230  1.00 23.64      A   C
ATOM   161  CG  ARG A  23      25.965  43.756  46.553  1.00 24.47      A   C
ATOM   162  CD  ARG A  23      26.093  42.252  46.372  1.00 30.28      A   C
ATOM   163  NE  ARG A  23      26.418  41.582  47.630  1.00 30.56      A   N
ATOM   164  CZ  ARG A  23      26.768  40.302  47.727  1.00 32.70      A   C
ATOM   165  NH1 ARG A  23      26.838  39.549  46.636  1.00 32.50      A   N
ATOM   166  NH2 ARG A  23      27.054  39.776  48.914  1.00 28.66      A   N
ATOM   167  C   ARG A  23      28.379  46.216  48.302  1.00 21.73      A   C
ATOM   168  O   ARG A  23      29.149  45.365  48.759  1.00 20.27      A   O
ATOM   169  N   LEU A  24      28.522  47.512  48.527  1.00 17.52      A   N
ATOM   170  CA  LEU A  24      29.624  48.018  49.317  1.00 21.03      A   C
ATOM   171  CB  LEU A  24      30.080  49.366  48.757  1.00 20.25      A   C
ATOM   172  CG  LEU A  24      30.478  49.366  47.282  1.00 22.97      A   C
ATOM   173  CD1 LEU A  24      30.723  50.797  46.810  1.00 22.12      A   C
ATOM   174  CD2 LEU A  24      31.723  48.510  47.094  1.00 21.35      A   C
ATOM   175  C   LEU A  24      29.239  48.184  50.776  1.00 21.90      A   C
ATOM   176  O   LEU A  24      30.079  48.032  51.663  1.00 23.97      A   O
ATOM   177  N   PHE A  25      27.968  48.483  51.028  1.00 20.73      A   N
ATOM   178  CA  PHE A  25      27.517  48.710  52.396  1.00 21.16      A   C
ATOM   179  CB  PHE A  25      27.290  50.207  52.609  1.00 19.75      A   C
ATOM   180  CG  PHE A  25      28.416  51.062  52.101  1.00 19.70      A   C
ATOM   181  CD1 PHE A  25      28.249  51.854  50.967  1.00 20.65      A   C
ATOM   182  CD2 PHE A  25      29.648  51.065  52.748  1.00 19.59      A   C
ATOM   183  CE1 PHE A  25      29.294  52.641  50.483  1.00 20.02      A   C
ATOM   184  CE2 PHE A  25      30.701  51.846  52.276  1.00 20.92      A   C
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Figure 4E

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ATOM   185 CZ  PHE A 25    30.522  52.639  51.137  1.00 19.72    A   C
ATOM   186 C   PHE A 25    26.259  47.940  52.773  1.00 18.19    A   C
ATOM   187 O   PHE A 25    25.387  47.718  51.945  1.00 20.08    A   O
ATOM   188 N   ASP A 26    26.174  47.562  54.044  1.00 19.15    A   N
ATOM   189 CA  ASP A 26    25.049  46.793  54.569  1.00 19.40    A   C
ATOM   190 CB  ASP A 26    25.524  45.978  55.768  1.00 21.39    A   C
ATOM   191 CG  ASP A 26    26.764  45.166  55.455  1.00 23.64    A   C
ATOM   192 OD1 ASP A 26    26.632  44.118  54.794  1.00 23.32    A   O
ATOM   193 OD2 ASP A 26    27.875  45.587  55.852  1.00 28.55    A   O
ATOM   194 C   ASP A 26    23.864  47.662  54.978  1.00 18.82    A   C
ATOM   195 O   ASP A 26    22.727  47.196  55.034  1.00 19.35    A   O
ATOM   196 N   GLU A 27    24.132  48.926  55.273  1.00 17.90    A   N
ATOM   197 CA  GLU A 27    23.067  49.840  55.671  1.00 17.07    A   C
ATOM   198 CB  GLU A 27    22.892  49.826  57.187  1.00 17.71    A   C
ATOM   199 CG  GLU A 27    21.646  50.550  57.663  1.00 24.75    A   C
ATOM   200 CD  GLU A 27    21.322  50.279  59.127  1.00 28.18    A   C
ATOM   201 OE1 GLU A 27    20.326  50.846  59.620  1.00 31.23    A   O
ATOM   202 OE2 GLU A 27    22.054  49.500  59.782  1.00 27.47    A   O
ATOM   203 C   GLU A 27    23.393  51.246  55.197  1.00 16.15    A   C
ATOM   204 O   GLU A 27    24.524  51.723  55.346  1.00 14.85    A   O
ATOM   205 N   ILE A 28    22.393  51.910  54.633  1.00 14.40    A   N
ATOM   206 CA  ILE A 28    22.577  53.257  54.118  1.00 12.75    A   C
ATOM   207 CB  ILE A 28    22.574  53.257  52.582  1.00 13.36    A   C
ATOM   208 CG2 ILE A 28    22.678  54.689  52.056  1.00  9.46    A   C
ATOM   209 CG1 ILE A 28    23.736  52.409  52.059  1.00 12.29    A   C
ATOM   210 CD1 ILE A 28    23.699  52.211  50.552  1.00 16.70    A   C
ATOM   211 C   ILE A 28    21.477  54.193  54.592  1.00 13.60    A   C
ATOM   212 O   ILE A 28    20.296  53.854  54.545  1.00 13.62    A   O
ATOM   213 N   ILE A 29    21.879  55.367  55.059  1.00 12.74    A   N
ATOM   214 CA  ILE A 29    20.928  56.375  55.507  1.00 14.14    A   C
ATOM   215 CB  ILE A 29    21.293  56.944  56.893  1.00 13.73    A   C
ATOM   216 CG2 ILE A 29    20.241  57.957  57.324  1.00 15.30    A   C
ATOM   217 CG1 ILE A 29    21.398  55.814  57.929  1.00 15.05    A   C
ATOM   218 CD1 ILE A 29    20.107  55.035  58.145  1.00 14.22    A   C
ATOM   219 C   ILE A 29    21.039  57.489  54.472  1.00 14.66    A   C
ATOM   220 O   ILE A 29    22.056  58.183  54.404  1.00 13.06    A   O
ATOM   221 N   TYR A 30    20.007  57.629  53.648  1.00 12.88    A   N
ATOM   222 CA  TYR A 30    19.987  58.649  52.609  1.00 14.23    A   C
ATOM   223 CB  TYR A 30    19.221  58.133  51.389  1.00 12.46    A   C
ATOM   224 CG  TYR A 30    19.221  59.075  50.205  1.00 15.02    A   C
ATOM   225 CD1 TYR A 30    20.155  58.933  49.178  1.00 12.86    A   C
ATOM   226 CE1 TYR A 30    20.171  59.803  48.088  1.00 12.85    A   C
ATOM   227 CD2 TYR A 30    18.298  60.119  50.117  1.00 15.96    A   C
ATOM   228 CE2 TYR A 30    18.304  60.996  49.034  1.00 15.05    A   C
ATOM   229 CZ  TYR A 30    19.243  60.831  48.023  1.00 14.12    A   C
ATOM   230 OH  TYR A 30    19.248  61.681  46.948  1.00 11.65    A   O
ATOM   231 C   TYR A 30    19.293  59.902  53.139  1.00 15.46    A   C
ATOM   232 O   TYR A 30    18.211  59.815  53.725  1.00 14.07    A   O
ATOM   233 N   TYR A 31    19.909  61.062  52.934  1.00 14.03    A   N
ATOM   234 CA  TYR A 31    19.297  62.312  53.370  1.00 14.37    A   C
ATOM   235 CB  TYR A 31    20.007  62.882  54.601  1.00 13.42    A   C
ATOM   236 CG  TYR A 31    19.441  64.216  55.045  1.00 13.73    A   C
ATOM   237 CD1 TYR A 31    18.150  64.307  55.559  1.00 15.42    A   C
ATOM   238 CE1 TYR A 31    17.616  65.532  55.962  1.00 18.80    A   C
ATOM   239 CD2 TYR A 31    20.191  65.389  54.940  1.00 15.22    A   C
ATOM   240 CE2 TYR A 31    19.665  66.625  55.335  1.00 19.27    A   C
ATOM   241 CZ  TYR A 31    18.376  66.686  55.847  1.00 20.56    A   C
ATOM   242 OH  TYR A 31    17.840  67.894  56.250  1.00 21.50    A   O
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Figure 4F

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ATOM   243  C   TYR A  31     19.321  63.355  52.257  1.00 13.94    A   C
ATOM   244  O   TYR A  31     20.383  63.704  51.743  1.00 12.53    A   O
ATOM   245  N   GLY A  32     18.139  63.836  51.876  1.00 14.52    A   N
ATOM   246  CA  GLY A  32     18.052  64.855  50.846  1.00 11.09    A   C
ATOM   247  C   GLY A  32     17.502  66.137  51.445  1.00 14.21    A   C
ATOM   248  O   GLY A  32     16.474  66.105  52.120  1.00 13.16    A   O
ATOM   249  N   ASP A  33     18.178  67.261  51.217  1.00 11.82    A   N
ATOM   250  CA  ASP A  33     17.728  68.550  51.754  1.00 12.90    A   C
ATOM   251  CB  ASP A  33     18.934  69.474  51.926  1.00 11.25    A   C
ATOM   252  CG  ASP A  33     18.576  70.788  52.587  1.00 11.81    A   C
ATOM   253  OD1 ASP A  33     17.562  70.842  53.309  1.00 14.26    A   O
ATOM   254  OD2 ASP A  33     19.326  71.757  52.394  1.00 11.68    A   O
ATOM   255  C   ASP A  33     16.703  69.145  50.783  1.00 13.65    A   C
ATOM   256  O   ASP A  33     16.824  70.285  50.324  1.00 12.95    A   O
ATOM   257  N   SER A  34     15.693  68.333  50.486  1.00 13.72    A   N
ATOM   258  CA  SER A  34     14.630  68.658  49.543  1.00 14.78    A   C
ATOM   259  CB  SER A  34     13.602  67.527  49.539  1.00 13.92    A   C
ATOM   260  OG  SER A  34     14.230  66.294  49.232  1.00 21.22    A   O
ATOM   261  C   SER A  34     13.914  69.980  49.751  1.00 16.62    A   C
ATOM   262  O   SER A  34     13.379  70.554  48.799  1.00 14.31    A   O
ATOM   263  N   ALA A  35     13.889  70.461  50.990  1.00 13.83    A   N
ATOM   264  CA  ALA A  35     13.216  71.717  51.282  1.00 14.72    A   C
ATOM   265  CB  ALA A  35     13.037  71.875  52.790  1.00 12.61    A   C
ATOM   266  C   ALA A  35     13.982  72.908  50.717  1.00 15.06    A   C
ATOM   267  O   ALA A  35     13.417  73.989  50.538  1.00 17.76    A   O
ATOM   268  N   ARG A  36     15.262  72.713  50.420  1.00 15.20    A   N
ATOM   269  CA  ARG A  36     16.076  73.804  49.902  1.00 15.09    A   C
ATOM   270  CB  ARG A  36     17.175  74.128  50.918  1.00 14.65    A   C
ATOM   271  CG  ARG A  36     16.585  74.462  52.284  1.00 13.95    A   C
ATOM   272  CD  ARG A  36     17.602  75.018  53.255  1.00 15.98    A   C
ATOM   273  NE  ARG A  36     18.579  74.020  53.681  1.00 14.55    A   N
ATOM   274  CZ  ARG A  36     19.333  74.141  54.769  1.00 19.35    A   C
ATOM   275  NH1 ARG A  36     19.217  75.221  55.537  1.00 16.64    A   N
ATOM   276  NH2 ARG A  36     20.201  73.187  55.093  1.00 16.02    A   N
ATOM   277  C   ARG A  36     16.668  73.578  48.511  1.00 15.81    A   C
ATOM   278  O   ARG A  36     17.422  74.409  48.002  1.00 15.67    A   O
ATOM   279  N   VAL A  37     16.319  72.461  47.888  1.00 15.48    A   N
ATOM   280  CA  VAL A  37     16.821  72.168  46.552  1.00 13.76    A   C
ATOM   281  CB  VAL A  37     16.374  70.746  46.115  1.00 14.93    A   C
ATOM   282  CG1 VAL A  37     14.877  70.727  45.851  1.00 14.99    A   C
ATOM   283  CG2 VAL A  37     17.174  70.280  44.898  1.00 14.00    A   C
ATOM   284  C   VAL A  37     16.246  73.243  45.617  1.00 11.66    A   C
ATOM   285  O   VAL A  37     15.112  73.697  45.805  1.00 11.22    A   O
ATOM   286  N   PRO A  38     17.011  73.662  44.596  1.00 12.05    A   N
ATOM   287  CD  PRO A  38     16.485  74.565  43.553  1.00 12.17    A   C
ATOM   288  CA  PRO A  38     18.356  73.214  44.244  1.00 13.67    A   C
ATOM   289  CB  PRO A  38     18.368  73.384  42.736  1.00 14.66    A   C
ATOM   290  CG  PRO A  38     17.655  74.698  42.588  1.00 12.08    A   C
ATOM   291  C   PRO A  38     19.486  74.000  44.898  1.00 15.15    A   C
ATOM   292  O   PRO A  38     19.297  75.129  45.370  1.00 12.96    A   O
ATOM   293  N   TYR A  39     20.664  73.382  44.900  1.00 11.07    A   N
ATOM   294  CA  TYR A  39     21.885  73.974  45.442  1.00 13.74    A   C
ATOM   295  CB  TYR A  39     22.796  72.893  46.040  1.00 11.65    A   C
ATOM   296  CG  TYR A  39     22.461  72.394  47.428  1.00 12.17    A   C
ATOM   297  CD1 TYR A  39     21.229  72.663  48.031  1.00 13.42    A   C
ATOM   298  CE1 TYR A  39     20.932  72.177  49.312  1.00 12.82    A   C
ATOM   299  CD2 TYR A  39     23.387  71.625  48.137  1.00 14.92    A   C
ATOM   300  CE2 TYR A  39     23.103  71.137  49.406  1.00 15.33    A   C
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Figure 4G

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ATOM   301 CZ  TYR A 39    21.878  71.414  49.992  1.00 13.34    A   C
ATOM   302 OH  TYR A 39    21.624  70.941  51.260  1.00 13.24    A   O
ATOM   303 C   TYR A 39    22.654  74.640  44.300  1.00 11.74    A   C
ATOM   304 O   TYR A 39    23.323  75.652  44.494  1.00 14.92    A   O
ATOM   305 N   GLY A 40    22.551  74.049  43.112  1.00 14.63    A   N
ATOM   306 CA  GLY A 40    23.269  74.529  41.939  1.00 12.47    A   C
ATOM   307 C   GLY A 40    23.196  75.993  41.544  1.00 14.09    A   C
ATOM   308 O   GLY A 40    24.093  76.502  40.871  1.00 12.63    A   O
ATOM   309 N   THR A 41    22.141  76.683  41.952  1.00 13.06    A   N
ATOM   310 CA  THR A 41    22.001  78.086  41.585  1.00 17.35    A   C
ATOM   311 CB  THR A 41    20.552  78.400  41.219  1.00 18.12    A   C
ATOM   312 OG1 THR A 41    19.713  78.078  42.332  1.00 22.00    A   O
ATOM   313 CG2 THR A 41    20.115  77.580  40.009  1.00 22.83    A   C
ATOM   314 C   THR A 41    22.416  79.020  42.712  1.00 16.33    A   C
ATOM   315 O   THR A 41    22.266  80.240  42.600  1.00 17.71    A   O
ATOM   316 N   LYS A 42    22.953  78.460  43.787  1.00 14.75    A   N
ATOM   317 CA  LYS A 42    23.331  79.281  44.922  1.00 13.75    A   C
ATOM   318 CB  LYS A 42    22.653  78.721  46.174  1.00 14.86    A   C
ATOM   319 CG  LYS A 42    21.139  78.899  46.078  1.00 14.53    A   C
ATOM   320 CD  LYS A 42    20.342  77.857  46.842  1.00 14.88    A   C
ATOM   321 CE  LYS A 42    18.898  77.878  46.349  1.00 13.95    A   C
ATOM   322 NZ  LYS A 42    17.995  76.929  47.073  1.00 12.60    A   N
ATOM   323 C   LYS A 42    24.824  79.496  45.119  1.00 16.57    A   C
ATOM   324 O   LYS A 42    25.647  78.943  44.391  1.00 14.82    A   O
ATOM   325 N   ASP A 43    25.157  80.329  46.099  1.00 17.21    A   N
ATOM   326 CA  ASP A 43    26.539  80.689  46.390  1.00 19.06    A   C
ATOM   327 CB  ASP A 43    26.567  82.117  46.932  1.00 20.48    A   C
ATOM   328 CG  ASP A 43    25.808  82.245  48.228  1.00 21.34    A   C
ATOM   329 OD1 ASP A 43    26.458  82.356  49.287  1.00 19.30    A   O
ATOM   330 OD2 ASP A 43    24.557  82.210  48.190  1.00 23.52    A   O
ATOM   331 C   ASP A 43    27.260  79.763  47.371  1.00 19.43    A   C
ATOM   332 O   ASP A 43    26.634  79.034  48.141  1.00 18.30    A   O
ATOM   333 N   PRO A 44    28.604  79.789  47.346  1.00 21.23    A   N
ATOM   334 CD  PRO A 44    29.401  80.567  46.377  1.00 20.65    A   C
ATOM   335 CA  PRO A 44    29.482  78.984  48.202  1.00 20.54    A   C
ATOM   336 CB  PRO A 44    30.866  79.543  47.886  1.00 20.91    A   C
ATOM   337 CG  PRO A 44    30.749  79.881  46.440  1.00 20.03    A   C
ATOM   338 C   PRO A 44    29.165  79.051  49.691  1.00 21.08    A   C
ATOM   339 O   PRO A 44    29.078  78.020  50.362  1.00 22.03    A   O
ATOM   340 N   THR A 45    28.999  80.266  50.207  1.00 20.06    A   N
ATOM   341 CA  THR A 45    28.707  80.453  51.622  1.00 19.83    A   C
ATOM   342 CB  THR A 45    28.523  81.953  51.961  1.00 22.19    A   C
ATOM   343 OG1 THR A 45    29.734  82.659  51.667  1.00 22.93    A   O
ATOM   344 CG2 THR A 45    28.180  82.135  53.429  1.00 21.29    A   C
ATOM   345 C   THR A 45    27.453  79.697  52.027  1.00 18.90    A   C
ATOM   346 O   THR A 45    27.448  78.950  53.007  1.00 16.82    A   O
ATOM   347 N   THR A 46    26.386  79.893  51.263  1.00 17.42    A   N
ATOM   348 CA  THR A 46    25.125  79.235  51.546  1.00 17.81    A   C
ATOM   349 CB  THR A 46    24.039  79.671  50.542  1.00 16.98    A   C
ATOM   350 OG1 THR A 46    23.835  81.087  50.636  1.00 17.53    A   O
ATOM   351 CG2 THR A 46    22.737  78.971  50.839  1.00 19.05    A   C
ATOM   352 C   THR A 46    25.265  77.719  51.484  1.00 17.51    A   C
ATOM   353 O   THR A 46    24.766  77.004  52.355  1.00 18.78    A   O
ATOM   354 N   ILE A 47    25.945  77.236  50.452  1.00 17.91    A   N
ATOM   355 CA  ILE A 47    26.134  75.803  50.265  1.00 20.81    A   C
ATOM   356 CB  ILE A 47    26.822  75.513  48.912  1.00 20.52    A   C
ATOM   357 CG2 ILE A 47    26.934  74.002  48.678  1.00 18.34    A   C
ATOM   358 CG1 ILE A 47    26.004  76.143  47.783  1.00 23.35    A   C
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Figure 4H

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ATOM   359 CD1 ILE A 47    24.523  75.792  47.826 1.00 23.82    A   C
ATOM   360 C   ILE A 47    26.935  75.170  51.398 1.00 19.27    A   C
ATOM   361 O   ILE A 47    26.568  74.111  51.905 1.00 21.96    A   O
ATOM   362 N   LYS A 48    28.018  75.818  51.805 1.00 21.30    A   N
ATOM   363 CA  LYS A 48    28.834  75.292  52.890 1.00 20.85    A   C
ATOM   364 CB  LYS A 48    30.032  76.203  53.151 1.00 22.83    A   C
ATOM   365 CG  LYS A 48    31.094  76.059  52.091 1.00 27.64    A   C
ATOM   366 CD  LYS A 48    32.380  76.794  52.444 1.00 31.38    A   C
ATOM   367 CE  LYS A 48    32.246  78.287  52.245 1.00 32.58    A   C
ATOM   368 NZ  LYS A 48    33.567  78.966  52.404 1.00 35.58    A   N
ATOM   369 C   LYS A 48    28.029  75.101  54.163 1.00 21.38    A   C
ATOM   370 O   LYS A 48    28.141  74.061  54.814 1.00 20.76    A   O
ATOM   371 N   GLN A 49    27.211  76.091  54.520 1.00 19.20    A   N
ATOM   372 CA  GLN A 49    26.395  75.963  55.716 1.00 19.40    A   C
ATOM   373 CB  GLN A 49    25.619  77.256  56.005 1.00 19.30    A   C
ATOM   374 CG  GLN A 49    24.776  77.203  57.286 1.00 22.44    A   C
ATOM   375 CD  GLN A 49    25.581  76.812  58.525 1.00 20.73    A   C
ATOM   376 OE1 GLN A 49    26.740  77.192  58.667 1.00 22.79    A   O
ATOM   377 NE2 GLN A 49    24.958  76.068  59.433 1.00 22.60    A   N
ATOM   378 C   GLN A 49    25.423  74.803  55.553 1.00 18.14    A   C
ATOM   379 O   GLN A 49    25.159  74.074  56.510 1.00 19.87    A   O
ATOM   380 N   PHE A 50    24.882  74.631  54.348 1.00 17.65    A   N
ATOM   381 CA  PHE A 50    23.960  73.521  54.112 1.00 17.56    A   C
ATOM   382 CB  PHE A 50    23.461  73.510  52.659 1.00 17.20    A   C
ATOM   383 CG  PHE A 50    22.478  74.604  52.331 1.00 18.53    A   C
ATOM   384 CD1 PHE A 50    21.961  75.433  53.323 1.00 18.95    A   C
ATOM   385 CD2 PHE A 50    22.041  74.780  51.022 1.00 20.21    A   C
ATOM   386 CE1 PHE A 50    21.023  76.418  53.022 1.00 19.32    A   C
ATOM   387 CE2 PHE A 50    21.101  75.763  50.709 1.00 22.48    A   C
ATOM   388 CZ  PHE A 50    20.592  76.583  51.716 1.00 21.15    A   C
ATOM   389 C   PHE A 50    24.706  72.217  54.401 1.00 15.70    A   C
ATOM   390 O   PHE A 50    24.178  71.311  55.048 1.00 15.38    A   O
ATOM   391 N   GLY A 51    25.945  72.143  53.922 1.00 18.19    A   N
ATOM   392 CA  GLY A 51    26.760  70.959  54.126 1.00 19.41    A   C
ATOM   393 C   GLY A 51    27.006  70.667  55.592 1.00 20.96    A   C
ATOM   394 O   GLY A 51    26.964  69.514  56.026 1.00 20.04    A   O
ATOM   395 N   LEU A 52    27.261  71.716  56.368 1.00 22.33    A   N
ATOM   396 CA  LEU A 52    27.508  71.542  57.791 1.00 22.23    A   C
ATOM   397 CB  LEU A 52    27.995  72.855  58.412 1.00 24.46    A   C
ATOM   398 CG  LEU A 52    29.385  73.328  57.980 1.00 25.92    A   C
ATOM   399 CD1 LEU A 52    29.734  74.618  58.719 1.00 28.98    A   C
ATOM   400 CD2 LEU A 52    30.423  72.249  58.293 1.00 27.40    A   C
ATOM   401 C   LEU A 52    26.246  71.063  58.493 1.00 21.84    A   C
ATOM   402 O   LEU A 52    26.294  70.180  59.344 1.00 21.12    A   O
ATOM   403 N   GLU A 53    25.107  71.635  58.124 1.00 20.72    A   N
ATOM   404 CA  GLU A 53    23.852  71.237  58.736 1.00 20.40    A   C
ATOM   405 CB  GLU A 53    22.731  72.185  58.294 1.00 21.74    A   C
ATOM   406 CG  GLU A 53    22.655  73.438  59.159 1.00 21.95    A   C
ATOM   407 CD  GLU A 53    21.839  74.551  58.536 1.00 23.86    A   C
ATOM   408 OE1 GLU A 53    20.797  74.260  57.906 1.00 23.19    A   O
ATOM   409 OE2 GLU A 53    22.238  75.727  58.685 1.00 24.44    A   O
ATOM   410 C   GLU A 53    23.514  69.789  58.405 1.00 19.46    A   C
ATOM   411 O   GLU A 53    22.813  69.122  59.160 1.00 22.12    A   O
ATOM   412 N   ALA A 54    24.022  69.295  57.282 1.00 20.85    A   N
ATOM   413 CA  ALA A 54    23.760  67.910  56.905 1.00 18.16    A   C
ATOM   414 CB  ALA A 54    24.252  67.647  55.498 1.00 16.88    A   C
ATOM   415 C   ALA A 54    24.474  66.997  57.899 1.00 18.85    A   C
ATOM   416 O   ALA A 54    23.953  65.944  58.280 1.00 18.10    A   O
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Figure 4I

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ATOM   417 N   LEU A 55    25.670 67.408 58.313 1.00 19.45    A   N
ATOM   418 CA  LEU A 55    26.442 66.639 59.281 1.00 19.66    A   C
ATOM   419 CB  LEU A 55    27.775 67.329 59.590 1.00 21.26    A   C
ATOM   420 CG  LEU A 55    28.782 67.408 58.442 1.00 22.31    A   C
ATOM   421 CD1 LEU A 55    30.070 68.042 58.935 1.00 21.17    A   C
ATOM   422 CD2 LEU A 55    29.055 66.008 57.898 1.00 22.77    A   C
ATOM   423 C   LEU A 55    25.626 66.504 60.556 1.00 21.84    A   C
ATOM   424 O   LEU A 55    25.589 65.437 61.166 1.00 20.58    A   O
ATOM   425 N   ASP A 56    24.959 67.584 60.953 1.00 21.85    A   N
ATOM   426 CA  ASP A 56    24.147 67.543 62.157 1.00 22.53    A   C
ATOM   427 CB  ASP A 56    23.506 68.904 62.437 1.00 25.87    A   C
ATOM   428 CG  ASP A 56    24.530 69.986 62.715 1.00 29.28    A   C
ATOM   429 OD1 ASP A 56    25.636 69.651 63.190 1.00 31.33    A   O
ATOM   430 OD2 ASP A 56    24.226 71.172 62.473 1.00 32.07    A   O
ATOM   431 C   ASP A 56    23.062 66.492 62.023 1.00 22.75    A   C
ATOM   432 O   ASP A 56    22.777 65.762 62.974 1.00 22.74    A   O
ATOM   433 N   PHE A 57    22.459 66.403 60.841 1.00 20.21    A   N
ATOM   434 CA  PHE A 57    21.404 65.422 60.633 1.00 21.09    A   C
ATOM   435 CB  PHE A 57    20.831 65.497 59.215 1.00 21.92    A   C
ATOM   436 CG  PHE A 57    19.915 64.352 58.893 1.00 21.43    A   C
ATOM   437 CD1 PHE A 57    18.609 64.336 59.370 1.00 22.87    A   C
ATOM   438 CD2 PHE A 57    20.393 63.233 58.214 1.00 20.64    A   C
ATOM   439 CE1 PHE A 57    17.792 63.218 59.184 1.00 20.01    A   C
ATOM   440 CE2 PHE A 57    19.589 62.112 58.024 1.00 21.14    A   C
ATOM   441 CZ  PHE A 57    18.286 62.104 58.512 1.00 23.52    A   C
ATOM   442 C   PHE A 57    21.873 63.991 60.864 1.00 18.61    A   C
ATOM   443 O   PHE A 57    21.148 63.181 61.441 1.00 20.52    A   O
ATOM   444 N   PHE A 58    23.081 63.679 60.408 1.00 19.51    A   N
ATOM   445 CA  PHE A 58    23.615 62.324 60.532 1.00 21.64    A   C
ATOM   446 CB  PHE A 58    24.701 62.097 59.478 1.00 18.15    A   C
ATOM   447 CG  PHE A 58    24.181 62.018 58.072 1.00 17.07    A   C
ATOM   448 CD1 PHE A 58    24.380 63.072 57.180 1.00 15.61    A   C
ATOM   449 CD2 PHE A 58    23.508 60.878 57.628 1.00 16.58    A   C
ATOM   450 CE1 PHE A 58    23.920 62.993 55.868 1.00 16.17    A   C
ATOM   451 CE2 PHE A 58    23.044 60.790 56.318 1.00 20.24    A   C
ATOM   452 CZ  PHE A 58    23.251 61.850 55.436 1.00 14.25    A   C
ATOM   453 C   PHE A 58    24.164 61.894 61.896 1.00 24.25    A   C
ATOM   454 O   PHE A 58    24.323 60.697 62.147 1.00 24.91    A   O
ATOM   455 N   LYS A 59    24.449 62.850 62.774 1.00 26.87    A   N
ATOM   456 CA  LYS A 59    25.014 62.528 64.087 1.00 28.83    A   C
ATOM   457 CB  LYS A 59    25.116 63.800 64.931 1.00 31.02    A   C
ATOM   458 CG  LYS A 59    26.127 64.792 64.374 1.00 33.56    A   C
ATOM   459 CD  LYS A 59    26.237 66.047 65.221 1.00 37.86    A   C
ATOM   460 CE  LYS A 59    27.270 67.000 64.632 1.00 38.94    A   C
ATOM   461 NZ  LYS A 59    27.433 68.240 65.443 1.00 41.75    A   N
ATOM   462 C   LYS A 59    24.312 61.419 64.879 1.00 28.21    A   C
ATOM   463 O   LYS A 59    24.973 60.541 65.439 1.00 28.12    A   O
ATOM   464 N   PRO A 60    22.969 61.437 64.933 1.00 27.85    A   N
ATOM   465 CD  PRO A 60    22.061 62.472 64.412 1.00 27.44    A   C
ATOM   466 CA  PRO A 60    22.219 60.409 65.671 1.00 26.21    A   C
ATOM   467 CB  PRO A 60    20.791 60.962 65.691 1.00 28.29    A   C
ATOM   468 CG  PRO A 60    20.961 62.446 65.419 1.00 29.74    A   C
ATOM   469 C   PRO A 60    22.264 59.040 64.994 1.00 25.09    A   C
ATOM   470 O   PRO A 60    22.116 58.004 65.640 1.00 24.61    A   O
ATOM   471 N   HIS A 61    22.469 59.045 63.682 1.00 24.30    A   N
ATOM   472 CA  HIS A 61    22.489 57.815 62.906 1.00 23.28    A   C
ATOM   473 CB  HIS A 61    22.210 58.148 61.445 1.00 23.75    A   C
ATOM   474 CG  HIS A 61    20.813 58.616 61.202 1.00 23.81    A   C
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Figure 4J

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ATOM   475  CD2 HIS A  61      20.307  59.858  61.017  1.00 24.28      A   C
ATOM   476  ND1 HIS A  61      19.738  57.753  61.163  1.00 21.57      A   N
ATOM   477  CE1 HIS A  61      18.631  58.443  60.963  1.00 21.88      A   C
ATOM   478  NE2 HIS A  61      18.948  59.723  60.871  1.00 24.37      A   N
ATOM   479  C   HIS A  61     23.754  56.979  63.012  1.00 23.45      A   C
ATOM   480  O   HIS A  61     23.812  55.879  62.475  1.00 23.17      A   O
ATOM   481  N   GLU A  62     24.752  57.497  63.718  1.00 26.52      A   N
ATOM   482  CA  GLU A  62      26.030  56.811  63.892  1.00 27.77      A   C
ATOM   483  CB  GLU A  62      25.944  55.818  65.062  1.00 33.97      A   C
ATOM   484  CG  GLU A  62      24.861  54.754  64.943  1.00 37.16      A   C
ATOM   485  CD  GLU A  62      24.468  54.176  66.292  1.00 40.46      A   C
ATOM   486  OE1 GLU A  62      25.367  53.907  67.117  1.00 41.12      A   O
ATOM   487  OE2 GLU A  62      23.255  53.983  66.525  1.00 42.43      A   O
ATOM   488  C   GLU A  62     26.545  56.118  62.626  1.00 26.21      A   C
ATOM   489  O   GLU A  62     26.699  54.897  62.579  1.00 26.16      A   O
ATOM   490  N   ILE A  63     26.798  56.913  61.591  1.00 22.24      A   N
ATOM   491  CA  ILE A  63      27.333  56.385  60.338  1.00 21.10      A   C
ATOM   492  CB  ILE A  63      26.904  57.246  59.124  1.00 19.78      A   C
ATOM   493  CG2 ILE A  63      25.416  57.065  58.859  1.00 15.78      A   C
ATOM   494  CG1 ILE A  63      27.224  58.718  59.388  1.00 16.88      A   C
ATOM   495  CD1 ILE A  63      27.000  59.636  58.189  1.00 18.48      A   C
ATOM   496  C   ILE A  63     28.853  56.420  60.483  1.00 18.95      A   C
ATOM   497  O   ILE A  63     29.385  57.182  61.293  1.00 19.85      A   O
ATOM   498  N   GLU A  64     29.553  55.593  59.718  1.00 19.95      A   N
ATOM   499  CA  GLU A  64     31.008  55.561  59.804  1.00 19.49      A   C
ATOM   500  CB  GLU A  64      31.492  54.118  59.926  1.00 22.43      A   C
ATOM   501  CG  GLU A  64      31.139  53.498  61.268  1.00 26.80      A   C
ATOM   502  CD  GLU A  64      31.762  52.136  61.452  1.00 29.61      A   C
ATOM   503  OE1 GLU A  64      33.012  52.044  61.421  1.00 31.41      A   O
ATOM   504  OE2 GLU A  64      31.003  51.160  61.623  1.00 29.53      A   O
ATOM   505  C   GLU A  64     31.684  56.251  58.630  1.00 17.37      A   C
ATOM   506  O   GLU A  64     32.890  56.453  58.631  1.00 16.28      A   O
ATOM   507  N   LEU A  65     30.890  56.615  57.632  1.00 18.28      A   N
ATOM   508  CA  LEU A  65      31.393  57.308  56.456  1.00 17.15      A   C
ATOM   509  CB  LEU A  65      32.035  56.318  55.478  1.00 18.66      A   C
ATOM   510  CG  LEU A  65      32.582  56.903  54.169  1.00 21.47      A   C
ATOM   511  CD1 LEU A  65      33.667  55.991  53.603  1.00 23.00      A   C
ATOM   512  CD2 LEU A  65      31.449  57.086  53.167  1.00 22.69      A   C
ATOM   513  C   LEU A  65     30.230  58.021  55.786  1.00 16.52      A   C
ATOM   514  O   LEU A  65     29.100  57.539  55.813  1.00 14.91      A   O
ATOM   515  N   LEU A  66     30.510  59.180  55.204  1.00 14.90      A   N
ATOM   516  CA  LEU A  66      29.486  59.946  54.526  1.00 14.23      A   C
ATOM   517  CB  LEU A  66      29.264  61.288  55.231  1.00 14.12      A   C
ATOM   518  CG  LEU A  66      28.297  62.240  54.514  1.00 14.20      A   C
ATOM   519  CD1 LEU A  66      26.932  61.586  54.415  1.00 14.73      A   C
ATOM   520  CD2 LEU A  66      28.195  63.562  55.262  1.00 13.86      A   C
ATOM   521  C   LEU A  66     29.864  60.200  53.077  1.00 14.92      A   C
ATOM   522  O   LEU A  66     30.975  60.642  52.773  1.00 14.96      A   O
ATOM   523  N   ILE A  67     28.938  59.886  52.181  1.00 13.46      A   N
ATOM   524  CA  ILE A  67      29.140  60.124  50.766  1.00 12.96      A   C
ATOM   525  CB  ILE A  67      28.641  58.953  49.886  1.00 13.86      A   C
ATOM   526  CG2 ILE A  67      28.617  59.385  48.419  1.00 12.97      A   C
ATOM   527  CG1 ILE A  67      29.541  57.729  50.066  1.00 14.37      A   C
ATOM   528  CD1 ILE A  67      29.105  56.530  49.237  1.00 18.27      A   C
ATOM   529  C   ILE A  67     28.314  61.346  50.406  1.00 12.36      A   C
ATOM   530  O   ILE A  67      27.116  61.420  50.719  1.00 13.82      A   O
ATOM   531  N   VAL A  68      28.964  62.317  49.780  1.00 12.37      A   N
ATOM   532  CA  VAL A  68      28.275  63.516  49.342  1.00 12.34      A   C
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Figure 4K

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ATOM   533 CB  VAL A  68     29.160  64.759  49.466  1.00 10.71    A   C
ATOM   534 CG1 VAL A  68     28.413  65.977  48.916  1.00 10.16    A   C
ATOM   535 CG2 VAL A  68     29.525  64.978  50.927  1.00 11.52    A   C
ATOM   536 C   VAL A  68     28.002  63.222  47.884  1.00 11.20    A   C
ATOM   537 O   VAL A  68     28.885  63.362  47.038  1.00 12.44    A   O
ATOM   538 N   ALA A  69     26.785  62.775  47.602  1.00  9.18    A   N
ATOM   539 CA  ALA A  69     26.405  62.415  46.244  1.00 10.89    A   C
ATOM   540 CB  ALA A  69     25.129  61.581  46.263  1.00  9.29    A   C
ATOM   541 C   ALA A  69     26.218  63.631  45.358  1.00 10.34    A   C
ATOM   542 O   ALA A  69     26.341  63.546  44.139  1.00 11.20    A   O
ATOM   543 N   CYS A  70     25.905  64.760  45.982  1.00 10.65    A   N
ATOM   544 CA  CYS A  70     25.692  66.000  45.253  1.00 11.99    A   C
ATOM   545 CB  CYS A  70     25.026  67.030  46.167  1.00 13.56    A   C
ATOM   546 SG  CYS A  70     24.697  68.605  45.370  1.00 10.79    A   S
ATOM   547 C   CYS A  70     27.004  66.560  44.720  1.00 11.25    A   C
ATOM   548 O   CYS A  70     27.981  66.708  45.463  1.00  9.23    A   O
ATOM   549 N   ASN A  71     27.030  66.867  43.425  1.00 10.81    A   N
ATOM   550 CA  ASN A  71     28.228  67.424  42.807  1.00  9.85    A   C
ATOM   551 CB  ASN A  71     28.120  67.369  41.285  1.00  7.25    A   C
ATOM   552 CG  ASN A  71     28.026  65.959  40.768  1.00  9.24    A   C
ATOM   553 OD1 ASN A  71     26.998  65.298  40.919  1.00  8.82    A   O
ATOM   554 ND2 ASN A  71     29.107  65.478  40.165  1.00  9.13    A   N
ATOM   555 C   ASN A  71     28.434  68.866  43.246  1.00 12.09    A   C
ATOM   556 O   ASN A  71     29.565  69.321  43.432  1.00  9.50    A   O
ATOM   557 N   THR A  72     27.337  69.593  43.399  1.00 10.94    A   N
ATOM   558 CA  THR A  72     27.436  70.975  43.834  1.00 10.39    A   C
ATOM   559 CB  THR A  72     26.073  71.676  43.779  1.00  9.07    A   C
ATOM   560 OG1 THR A  72     25.599  71.675  42.429  1.00 10.15    A   O
ATOM   561 CG2 THR A  72     26.200  73.122  44.262  1.00  9.53    A   C
ATOM   562 C   THR A  72     27.974  71.029  45.259  1.00 11.47    A   C
ATOM   563 O   THR A  72     28.882  71.808  45.556  1.00  9.49    A   O
ATOM   564 N   ALA A  73     27.415  70.202  46.144  1.00 13.67    A   N
ATOM   565 CA  ALA A  73     27.871  70.171  47.531  1.00 13.27    A   C
ATOM   566 CB  ALA A  73     26.979  69.251  48.368  1.00 15.12    A   C
ATOM   567 C   ALA A  73     29.318  69.691  47.586  1.00 15.74    A   C
ATOM   568 O   ALA A  73     30.111  70.160  48.412  1.00 15.99    A   O
ATOM   569 N   SER A  74     29.660  68.746  46.714  1.00 13.48    A   N
ATOM   570 CA  SER A  74     31.021  68.226  46.677  1.00 13.55    A   C
ATOM   571 CB  SER A  74     31.133  67.078  45.666  1.00 10.32    A   C
ATOM   572 OG  SER A  74     30.483  65.916  46.148  1.00 14.22    A   O
ATOM   573 C   SER A  74     31.994  69.333  46.297  1.00 15.60    A   C
ATOM   574 O   SER A  74     33.093  69.439  46.845  1.00 14.18    A   O
ATOM   575 N   ALA A  75     31.578  70.169  45.359  1.00 13.93    A   N
ATOM   576 CA  ALA A  75     32.422  71.259  44.899  1.00 15.79    A   C
ATOM   577 CB  ALA A  75     31.899  71.773  43.560  1.00 16.15    A   C
ATOM   578 C   ALA A  75     32.549  72.420  45.886  1.00 17.44    A   C
ATOM   579 O   ALA A  75     33.639  72.967  46.063  1.00 18.83    A   O
ATOM   580 N   LEU A  76     31.453  72.777  46.548  1.00 15.33    A   N
ATOM   581 CA  LEU A  76     31.462  73.920  47.460  1.00 17.71    A   C
ATOM   582 CB  LEU A  76     30.236  74.793  47.189  1.00 16.64    A   C
ATOM   583 CG  LEU A  76     30.154  75.642  45.917  1.00 19.98    A   C
ATOM   584 CD1 LEU A  76     30.338  74.793  44.681  1.00 15.78    A   C
ATOM   585 CD2 LEU A  76     28.801  76.343  45.886  1.00 19.48    A   C
ATOM   586 C   LEU A  76     31.544  73.693  48.967  1.00 18.84    A   C
ATOM   587 O   LEU A  76     32.101  74.531  49.685  1.00 17.49    A   O
ATOM   588 N   ALA A  77     30.996  72.584  49.456  1.00 16.91    A   N
ATOM   589 CA  ALA A  77     30.986  72.338  50.896  1.00 17.45    A   C
ATOM   590 CB  ALA A  77     29.546  72.118  51.363  1.00 15.97    A   C
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Figure 4L

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ATOM   591  C   ALA A  77     31.862  71.206  51.422  1.00 17.05      A   C
ATOM   592  O   ALA A  77     32.092  71.120  52.630  1.00 15.31      A   O
ATOM   593  N   LEU A  78     32.355  70.350  50.533  1.00 17.95      A   N
ATOM   594  CA  LEU A  78     33.173  69.217  50.950  1.00 18.28      A   C
ATOM   595  CB  LEU A  78     33.701  68.456  49.726  1.00 17.49      A   C
ATOM   596  CG  LEU A  78     34.425  67.141  50.053  1.00 18.47      A   C
ATOM   597  CD1 LEU A  78     33.467  66.196  50.771  1.00 13.07      A   C
ATOM   598  CD2 LEU A  78     34.949  66.493  48.772  1.00 15.57      A   C
ATOM   599  C   LEU A  78     34.337  69.572  51.873  1.00 19.44      A   C
ATOM   600  O   LEU A  78     34.478  68.986  52.944  1.00 17.85      A   O
ATOM   601  N   GLU A  79     35.173  70.524  51.472  1.00 20.74      A   N
ATOM   602  CA  GLU A  79     36.310  70.897  52.304  1.00 23.29      A   C
ATOM   603  CB  GLU A  79     37.112  72.023  51.652  1.00 25.50      A   C
ATOM   604  CG  GLU A  79     38.332  72.435  52.464  1.00 32.40      A   C
ATOM   605  CD  GLU A  79     39.248  73.382  51.714  1.00 36.37      A   C
ATOM   606  OE1 GLU A  79     38.811  74.501  51.377  1.00 38.33      A   O
ATOM   607  OE2 GLU A  79     40.411  73.002  51.459  1.00 40.30      A   O
ATOM   608  C   GLU A  79     35.900  71.312  53.716  1.00 22.08      A   C
ATOM   609  O   GLU A  79     36.512  70.888  54.691  1.00 22.83      A   O
ATOM   610  N   GLU A  80     34.862  72.132  53.825  1.00 22.05      A   N
ATOM   611  CA  GLU A  80     34.399  72.591  55.125  1.00 21.68      A   C
ATOM   612  CB  GLU A  80     33.336  73.675  54.957  1.00 26.13      A   C
ATOM   613  CG  GLU A  80     33.081  74.457  56.232  1.00 32.22      A   C
ATOM   614  CD  GLU A  80     34.173  75.479  56.521  1.00 34.38      A   C
ATOM   615  OE1 GLU A  80     35.371  75.145  56.399  1.00 36.64      A   O
ATOM   616  OE2 GLU A  80     33.828  76.623  56.878  1.00 38.94      A   O
ATOM   617  C   GLU A  80     33.823  71.435  55.939  1.00 21.19      A   C
ATOM   618  O   GLU A  80     34.013  71.359  57.152  1.00 20.49      A   O
ATOM   619  N   MET A  81     33.116  70.533  55.269  1.00 18.90      A   N
ATOM   620  CA  MET A  81     32.531  69.389  55.950  1.00 16.84      A   C
ATOM   621  CB  MET A  81     31.639  68.605  54.992  1.00 14.00      A   C
ATOM   622  CG  MET A  81     30.375  69.349  54.615  1.00 15.86      A   C
ATOM   623  SD  MET A  81     29.517  68.583  53.244  1.00 15.74      A   S
ATOM   624  CE  MET A  81     28.866  67.134  54.019  1.00 14.04      A   C
ATOM   625  C   MET A  81     33.618  68.474  56.503  1.00 17.31      A   C
ATOM   626  O   MET A  81     33.539  68.020  57.646  1.00 16.49      A   O
ATOM   627  N   GLN A  82     34.632  68.216  55.684  1.00 18.90      A   N
ATOM   628  CA  GLN A  82     35.739  67.351  56.078  1.00 22.12      A   C
ATOM   629  CB  GLN A  82     36.674  67.125  54.887  1.00 22.92      A   C
ATOM   630  CG  GLN A  82     36.001  66.442  53.706  1.00 21.03      A   C
ATOM   631  CD  GLN A  82     36.961  66.158  52.575  1.00 22.15      A   C
ATOM   632  OE1 GLN A  82     37.725  67.033  52.159  1.00 22.13      A   O
ATOM   633  NE2 GLN A  82     36.924  64.934  52.061  1.00 20.69      A   N
ATOM   634  C   GLN A  82     36.516  67.956  57.237  1.00 24.53      A   C
ATOM   635  O   GLN A  82     37.051  67.239  58.086  1.00 23.68      A   O
ATOM   636  N   LYS A  83     36.565  69.282  57.271  1.00 26.24      A   N
ATOM   637  CA  LYS A  83     37.282  69.993  58.317  1.00 30.03      A   C
ATOM   638  CB  LYS A  83     37.178  71.505  58.092  1.00 30.40      A   C
ATOM   639  CG  LYS A  83     38.023  72.336  59.041  1.00 34.26      A   C
ATOM   640  CD  LYS A  83     37.873  73.829  58.756  1.00 38.51      A   C
ATOM   641  CE  LYS A  83     38.287  74.175  57.329  1.00 42.25      A   C
ATOM   642  NZ  LYS A  83     38.067  75.619  57.005  1.00 43.57      A   N
ATOM   643  C   LYS A  83     36.764  69.650  59.708  1.00 30.42      A   C
ATOM   644  O   LYS A  83     37.551  69.395  60.616  1.00 31.77      A   O
ATOM   645  N   TYR A  84     35.445  69.624  59.870  1.00 30.72      A   N
ATOM   646  CA  TYR A  84     34.850  69.341  61.173  1.00 34.49      A   C
ATOM   647  CB  TYR A  84     33.702  70.322  61.441  1.00 38.58      A   C
ATOM   648  CG  TYR A  84     34.109  71.781  61.386  1.00 43.85      A   C
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Figure 4M

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ATOM   649 CD1 TYR A 84     34.172  72.465  60.169  1.00 45.26      A   C
ATOM   650 CE1 TYR A 84     34.575  73.803  60.111  1.00 46.74      A   C
ATOM   651 CD2 TYR A 84     34.460  72.472  62.549  1.00 45.80      A   C
ATOM   652 CE2 TYR A 84     34.865  73.808  62.501  1.00 47.25      A   C
ATOM   653 CZ  TYR A 84     34.920  74.467  61.281  1.00 47.45      A   C
ATOM   654 OH  TYR A 84     35.321  75.784  61.233  1.00 47.13      A   O
ATOM   655 C   TYR A 84     34.349  67.911  61.401  1.00 33.43      A   C
ATOM   656 O   TYR A 84     33.973  67.555  62.520  1.00 34.46      A   O
ATOM   657 N   SER A 85     34.348  67.088  60.361  1.00 30.46      A   N
ATOM   658 CA  SER A 85     33.865  65.721  60.507  1.00 27.21      A   C
ATOM   659 CB  SER A 85     33.384  65.192  59.160  1.00 26.99      A   C
ATOM   660 OG  SER A 85     33.003  63.836  59.279  1.00 27.59      A   O
ATOM   661 C   SER A 85     34.883  64.745  61.088  1.00 25.50      A   C
ATOM   662 O   SER A 85     36.059  64.778  60.730  1.00 24.71      A   O
ATOM   663 N   LYS A 86     34.415  63.875  61.981  1.00 23.68      A   N
ATOM   664 CA  LYS A 86     35.265  62.868  62.609  1.00 23.93      A   C
ATOM   665 CB  LYS A 86     34.741  62.509  64.005  1.00 26.65      A   C
ATOM   666 CG  LYS A 86     34.774  63.644  65.028  1.00 31.69      A   C
ATOM   667 CD  LYS A 86     36.190  63.990  65.491  1.00 34.31      A   C
ATOM   668 CE  LYS A 86     37.015  64.657  64.401  1.00 35.72      A   C
ATOM   669 NZ  LYS A 86     38.359  65.087  64.902  1.00 41.28      A   N
ATOM   670 C   LYS A 86     35.308  61.607  61.752  1.00 22.61      A   C
ATOM   671 O   LYS A 86     36.192  60.765  61.914  1.00 23.21      A   O
ATOM   672 N   ILE A 87     34.337  61.462  60.857  1.00 19.67      A   N
ATOM   673 CA  ILE A 87     34.305  60.302  59.975  1.00 18.68      A   C
ATOM   674 CB  ILE A 87     32.896  59.681  59.888  1.00 18.75      A   C
ATOM   675 CG2 ILE A 87     32.510  59.090  61.233  1.00 18.89      A   C
ATOM   676 CG1 ILE A 87     31.887  60.742  59.433  1.00 21.06      A   C
ATOM   677 CD1 ILE A 87     30.508  60.187  59.086  1.00 18.90      A   C
ATOM   678 C   ILE A 87     34.720  60.751  58.585  1.00 16.98      A   C
ATOM   679 O   ILE A 87     34.614  61.932  58.248  1.00 16.62      A   O
ATOM   680 N   PRO A 88     35.219  59.822  57.761  1.00 17.72      A   N
ATOM   681 CD  PRO A 88     35.548  58.403  57.992  1.00 17.09      A   C
ATOM   682 CA  PRO A 88     35.616  60.247  56.418  1.00 17.99      A   C
ATOM   683 CB  PRO A 88     36.319  59.011  55.857  1.00 19.59      A   C
ATOM   684 CG  PRO A 88     35.648  57.872  56.587  1.00 18.28      A   C
ATOM   685 C   PRO A 88     34.411  60.672  55.577  1.00 19.00      A   C
ATOM   686 O   PRO A 88     33.318  60.125  55.711  1.00 17.80      A   O
ATOM   687 N   ILE A 89     34.622  61.668  54.726  1.00 19.35      A   N
ATOM   688 CA  ILE A 89     33.577  62.163  53.843  1.00 18.35      A   C
ATOM   689 CB  ILE A 89     33.171  63.613  54.196  1.00 18.03      A   C
ATOM   690 CG2 ILE A 89     32.157  64.136  53.185  1.00 16.99      A   C
ATOM   691 CG1 ILE A 89     32.562  63.641  55.598  1.00 18.30      A   C
ATOM   692 CD1 ILE A 89     32.020  64.990  56.011  1.00 26.25      A   C
ATOM   693 C   ILE A 89     34.134  62.108  52.429  1.00 17.01      A   C
ATOM   694 O   ILE A 89     35.206  62.646  52.144  1.00 18.36      A   O
ATOM   695 N   VAL A 90     33.406  61.435  51.551  1.00 15.45      A   N
ATOM   696 CA  VAL A 90     33.829  61.270  50.173  1.00 14.79      A   C
ATOM   697 CB  VAL A 90     33.899  59.779  49.806  1.00 14.33      A   C
ATOM   698 CG1 VAL A 90     34.409  59.605  48.389  1.00 12.10      A   C
ATOM   699 CG2 VAL A 90     34.804  59.055  50.796  1.00 15.51      A   C
ATOM   700 C   VAL A 90     32.858  61.957  49.234  1.00 14.94      A   C
ATOM   701 O   VAL A 90     31.658  61.702  49.283  1.00 15.20      A   O
ATOM   702 N   GLY A 91     33.391  62.830  48.387  1.00 13.93      A   N
ATOM   703 CA  GLY A 91     32.570  63.540  47.427  1.00 14.67      A   C
ATOM   704 C   GLY A 91     32.606  62.829  46.087  1.00 15.17      A   C
ATOM   705 O   GLY A 91     33.262  61.794  45.937  1.00 15.39      A   O
ATOM   706 N   VAL A 92     31.921  63.391  45.101  1.00 13.28      A   N
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Figure 4N

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ATOM   707 CA  VAL A  92     31.871  62.777  43.782  1.00 15.09    A   C
ATOM   708 CB  VAL A  92     30.434  62.762  43.243  1.00 14.78    A   C
ATOM   709 CG1 VAL A  92     29.629  61.703  43.977  1.00 14.03    A   C
ATOM   710 CG2 VAL A  92     29.793  64.135  43.412  1.00 10.70    A   C
ATOM   711 C   VAL A  92     32.770  63.405  42.730  1.00 14.63    A   C
ATOM   712 O   VAL A  92     32.739  63.006  41.567  1.00 17.71    A   O
ATOM   713 N   ILE A  93     33.578  64.378  43.128  1.00 15.55    A   N
ATOM   714 CA  ILE A  93     34.468  65.025  42.176  1.00 16.08    A   C
ATOM   715 CB  ILE A  93     34.684  66.497  42.561  1.00 16.56    A   C
ATOM   716 CG2 ILE A  93     35.653  67.169  41.589  1.00 11.15    A   C
ATOM   717 CG1 ILE A  93     33.329  67.210  42.555  1.00 17.56    A   C
ATOM   718 CD1 ILE A  93     33.385  68.627  43.056  1.00 24.35    A   C
ATOM   719 C   ILE A  93     35.812  64.304  42.032  1.00 15.47    A   C
ATOM   720 O   ILE A  93     36.180  63.904  40.926  1.00 14.93    A   O
ATOM   721 N   GLU A  94     36.536  64.118  43.132  1.00 16.92    A   N
ATOM   722 CA  GLU A  94     37.831  63.446  43.052  1.00 16.92    A   C
ATOM   723 CB  GLU A  94     38.471  63.305  44.434  1.00 20.92    A   C
ATOM   724 CG  GLU A  94     39.894  62.754  44.361  1.00 26.29    A   C
ATOM   725 CD  GLU A  94     40.576  62.678  45.713  1.00 32.62    A   C
ATOM   726 OE1 GLU A  94     40.310  61.723  46.474  1.00 35.02    A   O
ATOM   727 OE2 GLU A  94     41.377  63.588  46.019  1.00 37.91    A   O
ATOM   728 C   GLU A  94     37.745  62.067  42.399  1.00 16.23    A   C
ATOM   729 O   GLU A  94     38.594  61.710  41.578  1.00 12.72    A   O
ATOM   730 N   PRO A  95     36.728  61.263  42.765  1.00 14.67    A   N
ATOM   731 CD  PRO A  95     35.728  61.426  43.835  1.00 11.50    A   C
ATOM   732 CA  PRO A  95     36.612  59.933  42.154  1.00 13.49    A   C
ATOM   733 CB  PRO A  95     35.324  59.385  42.766  1.00 10.50    A   C
ATOM   734 CG  PRO A  95     35.340  59.990  44.132  1.00 13.67    A   C
ATOM   735 C   PRO A  95     36.552  59.995  40.628  1.00 13.36    A   C
ATOM   736 O   PRO A  95     37.111  59.144  39.942  1.00 13.11    A   O
ATOM   737 N   SER A  96     35.868  61.001  40.097  1.00 13.15    A   N
ATOM   738 CA  SER A  96     35.769  61.145  38.652  1.00 13.88    A   C
ATOM   739 CB  SER A  96     34.712  62.190  38.287  1.00 13.27    A   C
ATOM   740 OG  SER A  96     33.415  61.695  38.569  1.00 13.98    A   O
ATOM   741 C   SER A  96     37.121  61.532  38.062  1.00 16.13    A   C
ATOM   742 O   SER A  96     37.482  61.069  36.978  1.00 16.25    A   O
ATOM   743 N   ILE A  97     37.862  62.381  38.774  1.00 16.51    A   N
ATOM   744 CA  ILE A  97     39.181  62.807  38.318  1.00 16.84    A   C
ATOM   745 CB  ILE A  97     39.836  63.786  39.325  1.00 20.72    A   C
ATOM   746 CG2 ILE A  97     41.243  64.165  38.860  1.00 19.14    A   C
ATOM   747 CG1 ILE A  97     38.968  65.039  39.477  1.00 21.89    A   C
ATOM   748 CD1 ILE A  97     38.774  65.827  38.192  1.00 22.65    A   C
ATOM   749 C   ILE A  97     40.070  61.572  38.178  1.00 17.43    A   C
ATOM   750 O   ILE A  97     40.762  61.399  37.171  1.00 16.68    A   O
ATOM   751 N   LEU A  98     40.043  60.716  39.193  1.00 15.65    A   N
ATOM   752 CA  LEU A  98     40.840  59.498  39.182  1.00 18.16    A   C
ATOM   753 CB  LEU A  98     40.749  58.809  40.547  1.00 16.07    A   C
ATOM   754 CG  LEU A  98     41.359  59.641  41.682  1.00 15.84    A   C
ATOM   755 CD1 LEU A  98     41.069  58.980  43.020  1.00 13.47    A   C
ATOM   756 CD2 LEU A  98     42.866  59.788  41.466  1.00 19.12    A   C
ATOM   757 C   LEU A  98     40.374  58.563  38.063  1.00 17.77    A   C
ATOM   758 O   LEU A  98     41.199  57.934  37.389  1.00 16.62    A   O
ATOM   759 N   ALA A  99     39.058  58.485  37.859  1.00 16.23    A   N
ATOM   760 CA  ALA A  99     38.490  57.643  36.807  1.00 18.22    A   C
ATOM   761 CB  ALA A  99     36.962  57.767  36.788  1.00 20.22    A   C
ATOM   762 C   ALA A  99     39.065  58.077  35.462  1.00 17.90    A   C
ATOM   763 O   ALA A  99     39.496  57.246  34.658  1.00 17.01    A   O
ATOM   764 N   ILE A 100     39.067  59.386  35.226  1.00 15.73    A   N
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Figure 4O

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ATOM   765 CA  ILE A 100    39.601  59.939  33.987  1.00 17.26    A   C
ATOM   766 CB  ILE A 100    39.378  61.461  33.932  1.00 12.99    A   C
ATOM   767 CG2 ILE A 100    40.158  62.065  32.772  1.00 16.82    A   C
ATOM   768 CG1 ILE A 100    37.880  61.752  33.795  1.00 15.82    A   C
ATOM   769 CD1 ILE A 100    37.516  63.216  33.925  1.00 14.23    A   C
ATOM   770 C   ILE A 100    41.099  59.640  33.878  1.00 19.31    A   C
ATOM   771 O   ILE A 100    41.594  59.260  32.815  1.00 19.06    A   O
ATOM   772 N   LYS A 101    41.812  59.802  34.986  1.00 19.58    A   N
ATOM   773 CA  LYS A 101    43.246  59.543  35.019  1.00 22.07    A   C
ATOM   774 CB  LYS A 101    43.771  59.741  36.440  1.00 23.70    A   C
ATOM   775 CG  LYS A 101    45.273  59.581  36.595  1.00 28.63    A   C
ATOM   776 CD  LYS A 101    45.671  59.665  38.062  1.00 33.56    A   C
ATOM   777 CE  LYS A 101    47.180  59.570  38.245  1.00 36.39    A   C
ATOM   778 NZ  LYS A 101    47.894  60.739  37.649  1.00 38.26    A   N
ATOM   779 C   LYS A 101    43.538  58.117  34.551  1.00 23.93    A   C
ATOM   780 O   LYS A 101    44.472  57.882  33.780  1.00 23.77    A   O
ATOM   781 N   ARG A 102    42.723  57.174  35.010  1.00 23.37    A   N
ATOM   782 CA  ARG A 102    42.899  55.775  34.655  1.00 25.65    A   C
ATOM   783 CB  ARG A 102    42.096  54.870  35.593  1.00 25.41    A   C
ATOM   784 CG  ARG A 102    42.656  54.749  37.000  1.00 28.61    A   C
ATOM   785 CD  ARG A 102    41.926  53.657  37.782  1.00 31.73    A   C
ATOM   786 NE  ARG A 102    40.486  53.903  37.858  1.00 35.18    A   N
ATOM   787 CZ  ARG A 102    39.903  54.713  38.736  1.00 34.42    A   C
ATOM   788 NH1 ARG A 102    38.586  54.876  38.718  1.00 29.69    A   N
ATOM   789 NH2 ARG A 102    40.637  55.344  39.644  1.00 34.01    A   N
ATOM   790 C   ARG A 102    42.522  55.437  33.222  1.00 26.39    A   C
ATOM   791 O   ARG A 102    43.180  54.611  32.594  1.00 26.86    A   O
ATOM   792 N   GLN A 103    41.473  56.061  32.694  1.00 26.77    A   N
ATOM   793 CA  GLN A 103    41.067  55.733  31.331  1.00 27.82    A   C
ATOM   794 CB  GLN A 103    39.585  55.335  31.306  1.00 28.07    A   C
ATOM   795 CG  GLN A 103    38.661  56.210  32.116  1.00 31.66    A   C
ATOM   796 CD  GLN A 103    37.378  55.489  32.504  1.00 32.01    A   C
ATOM   797 OE1 GLN A 103    36.672  54.951  31.651  1.00 32.82    A   O
ATOM   798 NE2 GLN A 103    37.071  55.479  33.797  1.00 31.78    A   N
ATOM   799 C   GLN A 103    41.363  56.739  30.223  1.00 26.37    A   C
ATOM   800 O   GLN A 103    41.024  56.494  29.066  1.00 26.19    A   O
ATOM   801 N   VAL A 104    42.003  57.856  30.559  1.00 25.47    A   N
ATOM   802 CA  VAL A 104    42.342  58.855  29.550  1.00 24.55    A   C
ATOM   803 CB  VAL A 104    41.542  60.154  29.756  1.00 23.42    A   C
ATOM   804 CG1 VAL A 104    41.998  61.208  28.755  1.00 24.85    A   C
ATOM   805 CG2 VAL A 104    40.055  59.876  29.582  1.00 19.58    A   C
ATOM   806 C   VAL A 104    43.838  59.174  29.578  1.00 26.78    A   C
ATOM   807 O   VAL A 104    44.287  60.043  30.324  1.00 25.34    A   O
ATOM   808 N   GLU A 105    44.601  58.460  28.755  1.00 27.15    A   N
ATOM   809 CA  GLU A 105    46.045  58.641  28.679  1.00 28.29    A   C
ATOM   810 CB  GLU A 105    46.680  57.457  27.947  1.00 33.28    A   C
ATOM   811 CG  GLU A 105    46.743  56.183  28.771  1.00 42.55    A   C
ATOM   812 CD  GLU A 105    47.669  56.315  29.969  1.00 46.07    A   C
ATOM   813 OE1 GLU A 105    47.467  57.242  30.784  1.00 48.67    A   O
ATOM   814 OE2 GLU A 105    48.600  55.491  30.095  1.00 49.87    A   O
ATOM   815 C   GLU A 105    46.461  59.930  27.995  1.00 27.62    A   C
ATOM   816 O   GLU A 105    47.395  60.600  28.437  1.00 27.02    A   O
ATOM   817 N   ASP A 106    45.769  60.273  26.914  1.00 26.11    A   N
ATOM   818 CA  ASP A 106    46.079  61.485  26.164  1.00 25.35    A   C
ATOM   819 CB  ASP A 106    45.271  61.526  24.867  1.00 24.40    A   C
ATOM   820 CG  ASP A 106    45.714  62.641  23.932  1.00 25.06    A   C
ATOM   821 OD1 ASP A 106    46.302  63.640  24.404  1.00 25.51    A   O
ATOM   822 OD2 ASP A 106    45.458  62.522  22.718  1.00 25.51    A   O
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Figure 4P

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ATOM   823  C   ASP A 106     45.759  62.722  26.991  1.00 24.65      A   C
ATOM   824  O   ASP A 106     44.593  63.086  27.142  1.00 24.49      A   O
ATOM   825  N   LYS A 107     46.791  63.372  27.519  1.00 25.06      A   N
ATOM   826  CA  LYS A 107     46.593  64.570  28.327  1.00 24.62      A   C
ATOM   827  CB  LYS A 107     47.919  65.024  28.954  1.00 26.00      A   C
ATOM   828  CG  LYS A 107     48.506  64.047  29.972  1.00 28.40      A   C
ATOM   829  CD  LYS A 107     47.527  63.770  31.107  1.00 26.24      A   C
ATOM   830  CE  LYS A 107     48.086  62.757  32.090  1.00 30.72      A   C
ATOM   831  NZ  LYS A 107     47.086  62.398  33.133  1.00 34.82      A   N
ATOM   832  C   LYS A 107     46.000  65.708  27.503  1.00 24.04      A   C
ATOM   833  O   LYS A 107     45.538  66.706  28.054  1.00 25.01      A   O
ATOM   834  N   ASN A 108     46.014  65.555  26.182  1.00 24.07      A   N
ATOM   835  CA  ASN A 108     45.473  66.572  25.286  1.00 23.49      A   C
ATOM   836  CB  ASN A 108     46.390  66.750  24.073  1.00 23.91      A   C
ATOM   837  CG  ASN A 108     47.596  67.601  24.385  1.00 26.66      A   C
ATOM   838  OD1 ASN A 108     47.464  68.780  24.716  1.00 28.22      A   O
ATOM   839  ND2 ASN A 108     48.780  67.011  24.293  1.00 26.45      A   N
ATOM   840  C   ASN A 108     44.059  66.255  24.818  1.00 21.66      A   C
ATOM   841  O   ASN A 108     43.487  66.983  24.009  1.00 22.58      A   O
ATOM   842  N   ALA A 109     43.494  65.164  25.321  1.00 21.45      A   N
ATOM   843  CA  ALA A 109     42.137  64.793  24.946  1.00 20.49      A   C
ATOM   844  CB  ALA A 109     41.755  63.468  25.599  1.00 21.55      A   C
ATOM   845  C   ALA A 109     41.187  65.902  25.402  1.00 18.98      A   C
ATOM   846  O   ALA A 109     41.237  66.346  26.546  1.00 18.14      A   O
ATOM   847  N   PRO A 110     40.315  66.375  24.505  1.00 19.61      A   N
ATOM   848  CD  PRO A 110     40.090  65.997  23.100  1.00 20.78      A   C
ATOM   849  CA  PRO A 110     39.397  67.436  24.919  1.00 18.53      A   C
ATOM   850  CB  PRO A 110     38.762  67.872  23.606  1.00 18.56      A   C
ATOM   851  CG  PRO A 110     38.726  66.596  22.825  1.00 22.18      A   C
ATOM   852  C   PRO A 110     38.380  66.924  25.928  1.00 17.90      A   C
ATOM   853  O   PRO A 110     37.623  65.996  25.650  1.00 18.78      A   O
ATOM   854  N   ILE A 111     38.384  67.526  27.109  1.00 16.88      A   N
ATOM   855  CA  ILE A 111     37.461  67.137  28.165  1.00 16.87      A   C
ATOM   856  CB  ILE A 111     38.197  66.905  29.503  1.00 17.13      A   C
ATOM   857  CG2 ILE A 111     37.195  66.560  30.592  1.00 18.00      A   C
ATOM   858  CG1 ILE A 111     39.225  65.780  29.352  1.00 16.90      A   C
ATOM   859  CD1 ILE A 111     40.127  65.612  30.574  1.00 20.07      A   C
ATOM   860  C   ILE A 111     36.438  68.246  28.360  1.00 14.74      A   C
ATOM   861  O   ILE A 111     36.792  69.422  28.422  1.00 18.10      A   O
ATOM   862  N   LEU A 112     35.170  67.861  28.450  1.00 15.95      A   N
ATOM   863  CA  LEU A 112     34.086  68.814  28.646  1.00 15.98      A   C
ATOM   864  CB  LEU A 112     33.081  68.715  27.498  1.00 13.81      A   C
ATOM   865  CG  LEU A 112     31.755  69.460  27.703  1.00 17.30      A   C
ATOM   866  CD1 LEU A 112     32.000  70.958  27.834  1.00 12.50      A   C
ATOM   867  CD2 LEU A 112     30.832  69.165  26.524  1.00 17.57      A   C
ATOM   868  C   LEU A 112     33.379  68.527  29.966  1.00 15.50      A   C
ATOM   869  O   LEU A 112     32.823  67.445  30.158  1.00 14.25      A   O
ATOM   870  N   VAL A 113     33.394  69.507  30.864  1.00 15.54      A   N
ATOM   871  CA  VAL A 113     32.767  69.361  32.173  1.00 15.01      A   C
ATOM   872  CB  VAL A 113     33.614  70.035  33.278  1.00 16.33      A   C
ATOM   873  CG1 VAL A 113     33.011  69.752  34.653  1.00 12.34      A   C
ATOM   874  CG2 VAL A 113     35.053  69.538  33.208  1.00 15.51      A   C
ATOM   875  C   VAL A 113     31.390  70.006  32.178  1.00 15.47      A   C
ATOM   876  O   VAL A 113     31.257  71.197  31.901  1.00 15.67      A   O
ATOM   877  N   LEU A 114     30.370  69.215  32.494  1.00 14.67      A   N
ATOM   878  CA  LEU A 114     29.000  69.717  32.554  1.00 13.42      A   C
ATOM   879  CB  LEU A 114     28.074  68.836  31.716  1.00 13.87      A   C
ATOM   880  CG  LEU A 114     28.440  68.622  30.247  1.00 15.67      A   C
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Figure 4Q

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ATOM   881 CD1 LEU A 114    27.349 67.775 29.595 1.00 14.66    A   C
ATOM   882 CD2 LEU A 114    28.583 69.965 29.528 1.00 16.47    A   C
ATOM   883 C   LEU A 114    28.536 69.684 34.006 1.00 12.89    A   C
ATOM   884 O   LEU A 114    28.772 68.706 34.718 1.00 12.06    A   O
ATOM   885 N   GLY A 115    27.873 70.745 34.451 1.00 13.97    A   N
ATOM   886 CA  GLY A 115    27.403 70.763 35.822 1.00 12.19    A   C
ATOM   887 C   GLY A 115    26.528 71.961 36.088 1.00 13.28    A   C
ATOM   888 O   GLY A 115    26.171 72.696 35.160 1.00 14.73    A   O
ATOM   889 N   THR A 116    26.167 72.153 37.351 1.00 11.11    A   N
ATOM   890 CA  THR A 116    25.348 73.297 37.725 1.00 13.32    A   C
ATOM   891 CB  THR A 116    24.866 73.197 39.170 1.00 11.37    A   C
ATOM   892 OG1 THR A 116    26.000 73.180 40.041 1.00 10.70    A   O
ATOM   893 CG2 THR A 116    24.036 71.939 39.367 1.00 10.35    A   C
ATOM   894 C   THR A 116    26.195 74.554 37.614 1.00 14.14    A   C
ATOM   895 O   THR A 116    27.416 74.482 37.431 1.00 14.71    A   O
ATOM   896 N   LYS A 117    25.535 75.701 37.716 1.00 13.99    A   N
ATOM   897 CA  LYS A 117    26.204 76.993 37.657 1.00 14.71    A   C
ATOM   898 CB  LYS A 117    25.147 78.105 37.777 1.00 15.38    A   C
ATOM   899 CG  LYS A 117    25.652 79.472 38.236 1.00 25.83    A   C
ATOM   900 CD  LYS A 117    26.685 80.064 37.296 1.00 33.76    A   C
ATOM   901 CE  LYS A 117    26.103 80.361 35.920 1.00 38.20    A   C
ATOM   902 NZ  LYS A 117    27.105 81.002 35.015 1.00 42.09    A   N
ATOM   903 C   LYS A 117    27.233 77.085 38.787 1.00 12.72    A   C
ATOM   904 O   LYS A 117    28.356 77.549 38.588 1.00 11.82    A   O
ATOM   905 N   ALA A 118    26.854 76.621 39.972 1.00 11.59    A   N
ATOM   906 CA  ALA A 118    27.750 76.671 41.120 1.00 11.90    A   C
ATOM   907 CB  ALA A 118    26.990 76.297 42.382 1.00  8.77    A   C
ATOM   908 C   ALA A 118    28.965 75.758 40.955 1.00 13.39    A   C
ATOM   909 O   ALA A 118    30.099 76.161 41.223 1.00 14.34    A   O
ATOM   910 N   THR A 119    28.721 74.530 40.508 1.00 13.12    A   N
ATOM   911 CA  THR A 119    29.789 73.561 40.316 1.00 12.85    A   C
ATOM   912 CB  THR A 119    29.224 72.205 39.840 1.00 13.42    A   C
ATOM   913 OG1 THR A 119    28.398 71.647 40.869 1.00 11.57    A   O
ATOM   914 CG2 THR A 119    30.353 71.235 39.509 1.00 13.13    A   C
ATOM   915 C   THR A 119    30.808 74.050 39.298 1.00 12.99    A   C
ATOM   916 O   THR A 119    32.016 74.004 39.547 1.00 13.76    A   O
ATOM   917 N   ILE A 120    30.323 74.520 38.154 1.00 11.88    A   N
ATOM   918 CA  ILE A 120    31.213 75.003 37.105 1.00 13.74    A   C
ATOM   919 CB  ILE A 120    30.419 75.310 35.807 1.00 13.41    A   C
ATOM   920 CG2 ILE A 120    31.321 75.980 34.769 1.00 14.31    A   C
ATOM   921 CG1 ILE A 120    29.799 74.012 35.266 1.00 14.49    A   C
ATOM   922 CD1 ILE A 120    30.786 72.862 35.086 1.00 12.48    A   C
ATOM   923 C   ILE A 120    31.977 76.246 37.547 1.00 16.55    A   C
ATOM   924 O   ILE A 120    33.192 76.337 37.372 1.00 18.38    A   O
ATOM   925 N   GLN A 121    31.257 77.200 38.126 1.00 19.17    A   N
ATOM   926 CA  GLN A 121    31.861 78.437 38.601 1.00 20.47    A   C
ATOM   927 CB  GLN A 121    30.790 79.302 39.275 1.00 22.58    A   C
ATOM   928 CG  GLN A 121    31.332 80.406 40.175 1.00 27.23    A   C
ATOM   929 CD  GLN A 121    30.251 81.377 40.627 1.00 30.53    A   C
ATOM   930 OE1 GLN A 121    30.383 82.030 41.664 1.00 32.67    A   O
ATOM   931 NE2 GLN A 121    29.185 81.486 39.842 1.00 28.50    A   N
ATOM   932 C   GLN A 121    33.012 78.170 39.570 1.00 20.02    A   C
ATOM   933 O   GLN A 121    33.979 78.931 39.622 1.00 20.38    A   O
ATOM   934 N   SER A 122    32.905 77.082 40.326 1.00 20.65    A   N
ATOM   935 CA  SER A 122    33.919 76.709 41.311 1.00 19.01    A   C
ATOM   936 CB  SER A 122    33.377 75.609 42.222 1.00 17.57    A   C
ATOM   937 OG  SER A 122    33.446 74.356 41.556 1.00 13.49    A   O
ATOM   938 C   SER A 122    35.220 76.201 40.686 1.00 18.75    A   C
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Figure 4R

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ATOM   939  O   SER A 122     36.270  76.232  41.325  1.00 17.22      A   O
ATOM   940  N   ASN A 123     35.136  75.709  39.454  1.00 18.64      A   N
ATOM   941  CA  ASN A 123     36.292  75.159  38.752  1.00 19.81      A   C
ATOM   942  CB  ASN A 123     37.355  76.237  38.538  1.00 23.62      A   C
ATOM   943  CG  ASN A 123     36.915  77.277  37.537  1.00 27.79      A   C
ATOM   944  OD1 ASN A 123     36.375  76.939  36.483  1.00 25.00      A   O
ATOM   945  ND2 ASN A 123     37.141  78.549  37.855  1.00 30.06      A   N
ATOM   946  C   ASN A 123     36.898  73.967  39.487  1.00 18.35      A   C
ATOM   947  O   ASN A 123     38.057  73.606  39.272  1.00 15.93      A   O
ATOM   948  N   ALA A 124     36.101  73.356  40.356  1.00 16.83      A   N
ATOM   949  CA  ALA A 124     36.550  72.197  41.113  1.00 18.02      A   C
ATOM   950  CB  ALA A 124     35.392  71.613  41.914  1.00 17.02      A   C
ATOM   951  C   ALA A 124     37.109  71.148  40.157  1.00 16.55      A   C
ATOM   952  O   ALA A 124     38.195  70.614  40.376  1.00 17.86      A   O
ATOM   953  N   TYR A 125     36.370  70.858  39.091  1.00 15.55      A   N
ATOM   954  CA  TYR A 125     36.817  69.870  38.121  1.00 15.38      A   C
ATOM   955  CB  TYR A 125     35.699  69.549  37.125  1.00 14.36      A   C
ATOM   956  CG  TYR A 125     34.638  68.609  37.662  1.00 15.54      A   C
ATOM   957  CD1 TYR A 125     33.460  69.096  38.226  1.00 13.69      A   C
ATOM   958  CE1 TYR A 125     32.478  68.230  38.701  1.00 16.51      A   C
ATOM   959  CD2 TYR A 125     34.813  67.224  37.591  1.00 15.03      A   C
ATOM   960  CE2 TYR A 125     33.839  66.349  38.064  1.00 16.83      A   C
ATOM   961  CZ  TYR A 125     32.677  66.857  38.614  1.00 15.95      A   C
ATOM   962  OH  TYR A 125     31.718  65.993  39.065  1.00 16.50      A   O
ATOM   963  C   TYR A 125     38.060  70.323  37.361  1.00 15.65      A   C
ATOM   964  O   TYR A 125     39.050  69.596  37.289  1.00 12.18      A   O
ATOM   965  N   ASP A 126     37.998  71.523  36.796  1.00 15.04      A   N
ATOM   966  CA  ASP A 126     39.110  72.080  36.032  1.00 19.15      A   C
ATOM   967  CB  ASP A 126     38.805  73.530  35.642  1.00 18.87      A   C
ATOM   968  CG  ASP A 126     37.532  73.659  34.831  1.00 21.01      A   C
ATOM   969  OD1 ASP A 126     36.489  73.129  35.271  1.00 22.54      A   O
ATOM   970  OD2 ASP A 126     37.570  74.295  33.756  1.00 22.03      A   O
ATOM   971  C   ASP A 126     40.423  72.028  36.814  1.00 19.26      A   C
ATOM   972  O   ASP A 126     41.432  71.519  36.316  1.00 19.31      A   O
ATOM   973  N   ASN A 127     40.406  72.542  38.040  1.00 18.32      A   N
ATOM   974  CA  ASN A 127     41.613  72.549  38.860  1.00 20.39      A   C
ATOM   975  CB  ASN A 127     41.349  73.226  40.206  1.00 19.27      A   C
ATOM   976  CG  ASN A 127     41.031  74.703  40.067  1.00 23.43      A   C
ATOM   977  OD1 ASN A 127     41.553  75.382  39.185  1.00 25.20      A   O
ATOM   978  ND2 ASN A 127     40.185  75.213  40.955  1.00 22.93      A   N
ATOM   979  C   ASN A 127     42.183  71.155  39.096  1.00 19.69      A   C
ATOM   980  O   ASN A 127     43.381  70.926  38.926  1.00 19.93      A   O
ATOM   981  N   ALA A 128     41.325  70.222  39.488  1.00 17.80      A   N
ATOM   982  CA  ALA A 128     41.767  68.862  39.742  1.00 19.25      A   C
ATOM   983  CB  ALA A 128     40.596  68.016  40.218  1.00 17.14      A   C
ATOM   984  C   ALA A 128     42.383  68.253  38.489  1.00 18.99      A   C
ATOM   985  O   ALA A 128     43.434  67.614  38.553  1.00 21.03      A   O
ATOM   986  N   LEU A 129     41.734  68.456  37.347  1.00 18.35      A   N
ATOM   987  CA  LEU A 129     42.237  67.911  36.088  1.00 18.37      A   C
ATOM   988  CB  LEU A 129     41.229  68.157  34.966  1.00 16.99      A   C
ATOM   989  CG  LEU A 129     39.944  67.331  35.044  1.00 17.37      A   C
ATOM   990  CD1 LEU A 129     38.906  67.908  34.101  1.00 18.55      A   C
ATOM   991  CD2 LEU A 129     40.247  65.878  34.690  1.00 19.31      A   C
ATOM   992  C   LEU A 129     43.586  68.512  35.709  1.00 18.69      A   C
ATOM   993  O   LEU A 129     44.486  67.799  35.264  1.00 16.61      A   O
ATOM   994  N   LYS A 130     43.722  69.823  35.881  1.00 20.51      A   N
ATOM   995  CA  LYS A 130     44.974  70.492  35.559  1.00 25.95      A   C
ATOM   996  CB  LYS A 130     44.869  72.002  35.815  1.00 29.56      A   C
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Figure 4S

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ATOM   997 CG  LYS A 130    44.065  72.756  34.766 1.00 35.38    A   C
ATOM   998 CD  LYS A 130    44.211  74.273  34.910 1.00 40.67    A   C
ATOM   999 CE  LYS A 130    43.491  74.796  36.138 1.00 44.58    A   C
ATOM  1000 NZ  LYS A 130    42.021  74.573  36.036 1.00 48.51    A   N
ATOM  1001 C   LYS A 130    46.084  69.899  36.413 1.00 27.20    A   C
ATOM  1002 O   LYS A 130    47.173  69.607  35.921 1.00 26.83    A   O
ATOM  1003 N   GLN A 131    45.793  69.711  37.695 1.00 27.73    A   N
ATOM  1004 CA  GLN A 131    46.768  69.152  38.615 1.00 30.51    A   C
ATOM  1005 CB  GLN A 131    46.168  69.058  40.017 1.00 34.61    A   C
ATOM  1006 CG  GLN A 131    47.164  68.658  41.086 1.00 44.44    A   C
ATOM  1007 CD  GLN A 131    46.499  68.364  42.414 1.00 49.85    A   C
ATOM  1008 OE1 GLN A 131    45.721  67.415  42.532 1.00 53.57    A   O
ATOM  1009 NE2 GLN A 131    46.797  69.181  43.423 1.00 52.59    A   N
ATOM  1010 C   GLN A 131    47.205  67.769  38.139 1.00 29.59    A   C
ATOM  1011 O   GLN A 131    48.333  67.347  38.389 1.00 27.34    A   O
ATOM  1012 N   GLN A 132    46.311  67.066  37.452 1.00 27.34    A   N
ATOM  1013 CA  GLN A 132    46.634  65.738  36.950 1.00 28.50    A   C
ATOM  1014 CB  GLN A 132    45.382  64.865  36.894 1.00 30.13    A   C
ATOM  1015 CG  GLN A 132    44.863  64.445  38.253 1.00 32.88    A   C
ATOM  1016 CD  GLN A 132    45.924  63.758  39.093 1.00 36.97    A   C
ATOM  1017 OE1 GLN A 132    46.545  62.787  38.659 1.00 36.12    A   O
ATOM  1018 NE2 GLN A 132    46.136  64.262  40.308 1.00 36.40    A   N
ATOM  1019 C   GLN A 132    47.297  65.764  35.579 1.00 26.54    A   C
ATOM  1020 O   GLN A 132    47.465  64.721  34.948 1.00 25.99    A   O
ATOM  1021 N   GLY A 133    47.653  66.958  35.113 1.00 25.65    A   N
ATOM  1022 CA  GLY A 133    48.326  67.079  33.833 1.00 25.61    A   C
ATOM  1023 C   GLY A 133    47.496  67.252  32.575 1.00 26.98    A   C
ATOM  1024 O   GLY A 133    48.061  67.293  31.479 1.00 25.64    A   O
ATOM  1025 N   TYR A 134    46.174  67.353  32.696 1.00 25.10    A   N
ATOM  1026 CA  TYR A 134    45.357  67.526  31.495 1.00 24.59    A   C
ATOM  1027 CB  TYR A 134    43.902  67.120  31.762 1.00 20.44    A   C
ATOM  1028 CG  TYR A 134    43.781  65.626  31.951 1.00 19.78    A   C
ATOM  1029 CD1 TYR A 134    43.870  65.050  33.219 1.00 21.76    A   C
ATOM  1030 CE1 TYR A 134    43.868  63.664  33.380 1.00 19.57    A   C
ATOM  1031 CD2 TYR A 134    43.681  64.774  30.850 1.00 19.08    A   C
ATOM  1032 CE2 TYR A 134    43.682  63.389  31.002 1.00 17.24    A   C
ATOM  1033 CZ  TYR A 134    43.777  62.842  32.265 1.00 18.47    A   C
ATOM  1034 OH  TYR A 134    43.792  61.473  32.413 1.00 19.23    A   O
ATOM  1035 C   TYR A 134    45.461  68.951  30.972 1.00 22.87    A   C
ATOM  1036 O   TYR A 134    45.446  69.908  31.746 1.00 22.48    A   O
ATOM  1037 N   LEU A 135    45.571  69.078  29.650 1.00 22.86    A   N
ATOM  1038 CA  LEU A 135    45.750  70.377  29.008 1.00 24.08    A   C
ATOM  1039 CB  LEU A 135    47.048  70.359  28.192 1.00 24.76    A   C
ATOM  1040 CG  LEU A 135    48.311  69.857  28.906 1.00 25.95    A   C
ATOM  1041 CD1 LEU A 135    49.461  69.790  27.913 1.00 27.98    A   C
ATOM  1042 CD2 LEU A 135    48.658  70.779  30.068 1.00 26.13    A   C
ATOM  1043 C   LEU A 135    44.628  70.873  28.107 1.00 23.53    A   C
ATOM  1044 O   LEU A 135    44.736  71.957  27.539 1.00 24.90    A   O
ATOM  1045 N   ASN A 136    43.556  70.100  27.970 1.00 22.37    A   N
ATOM  1046 CA  ASN A 136    42.450  70.499  27.102 1.00 20.74    A   C
ATOM  1047 CB  ASN A 136    42.411  69.585  25.876 1.00 21.50    A   C
ATOM  1048 CG  ASN A 136    41.613  70.170  24.735 1.00 23.18    A   C
ATOM  1049 OD1 ASN A 136    40.590  70.822  24.945 1.00 25.29    A   O
ATOM  1050 ND2 ASN A 136    42.068  69.923  23.511 1.00 23.17    A   N
ATOM  1051 C   ASN A 136    41.146  70.370  27.887 1.00 20.55    A   C
ATOM  1052 O   ASN A 136    40.430  69.386  27.744 1.00 20.93    A   O
ATOM  1053 N   ILE A 137    40.847  71.371  28.709 1.00 19.65    A   N
ATOM  1054 CA  ILE A 137    39.649  71.347  29.545 1.00 19.51    A   C
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Figure 4T

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ATOM  1055  CB  ILE A 137     40.021  71.504  31.032  1.00 19.77    A   C
ATOM  1056  CG2 ILE A 137     38.792  71.235  31.905  1.00 18.91    A   C
ATOM  1057  CG1 ILE A 137     41.165  70.548  31.388  1.00 17.50    A   C
ATOM  1058  CD1 ILE A 137     41.841  70.877  32.705  1.00 17.99    A   C
ATOM  1059  C   ILE A 137     38.650  72.445  29.214  1.00 18.94    A   C
ATOM  1060  O   ILE A 137     39.008  73.618  29.141  1.00 18.47    A   O
ATOM  1061  N   SER A 138     37.394  72.054  29.019  1.00 18.59    A   N
ATOM  1062  CA  SER A 138     36.319  73.000  28.729  1.00 19.77    A   C
ATOM  1063  CB  SER A 138     35.810  72.829  27.294  1.00 21.73    A   C
ATOM  1064  OG  SER A 138     36.823  73.104  26.345  1.00 24.47    A   O
ATOM  1065  C   SER A 138     35.177  72.716  29.698  1.00 19.64    A   C
ATOM  1066  O   SER A 138     34.971  71.569  30.102  1.00 20.10    A   O
ATOM  1067  N   HIS A 139     34.443  73.753  30.083  1.00 18.51    A   N
ATOM  1068  CA  HIS A 139     33.319  73.565  30.993  1.00 18.98    A   C
ATOM  1069  CB  HIS A 139     33.697  73.982  32.418  1.00 18.17    A   C
ATOM  1070  CG  HIS A 139     34.220  75.380  32.522  1.00 19.94    A   C
ATOM  1071  CD2 HIS A 139     33.634  76.575  32.268  1.00 20.85    A   C
ATOM  1072  ND1 HIS A 139     35.506  75.661  32.926  1.00 20.98    A   N
ATOM  1073  CE1 HIS A 139     35.692  76.970  32.916  1.00 24.03    A   C
ATOM  1074  NE2 HIS A 139     34.572  77.547  32.520  1.00 22.03    A   N
ATOM  1075  C   HIS A 139     32.082  74.329  30.552  1.00 18.46    A   C
ATOM  1076  O   HIS A 139     32.181  75.372  29.909  1.00 19.58    A   O
ATOM  1077  N   LEU A 140     30.918  73.791  30.902  1.00 18.71    A   N
ATOM  1078  CA  LEU A 140     29.634  74.403  30.573  1.00 19.01    A   C
ATOM  1079  CB  LEU A 140     29.028  73.775  29.316  1.00 20.85    A   C
ATOM  1080  CG  LEU A 140     29.476  74.190  27.918  1.00 22.92    A   C
ATOM  1081  CD1 LEU A 140     28.667  73.394  26.904  1.00 21.79    A   C
ATOM  1082  CD2 LEU A 140     29.255  75.688  27.709  1.00 25.42    A   C
ATOM  1083  C   LEU A 140     28.632  74.227  31.702  1.00 17.69    A   C
ATOM  1084  O   LEU A 140     28.422  73.118  32.194  1.00 17.06    A   O
ATOM  1085  N   ALA A 141     28.008  75.322  32.112  1.00 18.99    A   N
ATOM  1086  CA  ALA A 141     26.995  75.256  33.153  1.00 18.92    A   C
ATOM  1087  CB  ALA A 141     26.976  76.553  33.955  1.00 19.92    A   C
ATOM  1088  C   ALA A 141     25.653  75.046  32.456  1.00 20.05    A   C
ATOM  1089  O   ALA A 141     25.002  76.007  32.053  1.00 22.92    A   O
ATOM  1090  N   THR A 142     25.250  73.790  32.299  1.00 17.67    A   N
ATOM  1091  CA  THR A 142     23.983  73.456  31.650  1.00 15.92    A   C
ATOM  1092  CB  THR A 142     24.069  72.061  30.991  1.00 15.55    A   C
ATOM  1093  OG1 THR A 142     24.474  71.094  31.969  1.00 15.28    A   O
ATOM  1094  CG2 THR A 142     25.091  72.069  29.862  1.00 16.16    A   C
ATOM  1095  C   THR A 142     22.890  73.462  32.725  1.00 16.51    A   C
ATOM  1096  O   THR A 142     22.195  72.469  32.942  1.00 15.07    A   O
ATOM  1097  N   SER A 143     22.746  74.608  33.382  1.00 15.40    A   N
ATOM  1098  CA  SER A 143     21.797  74.779  34.479  1.00 16.69    A   C
ATOM  1099  CB  SER A 143     21.745  76.254  34.886  1.00 18.40    A   C
ATOM  1100  OG  SER A 143     20.979  76.419  36.068  1.00 19.14    A   O
ATOM  1101  C   SER A 143     20.374  74.259  34.266  1.00 16.28    A   C
ATOM  1102  O   SER A 143     19.838  73.555  35.119  1.00 17.50    A   O
ATOM  1103  N   LEU A 144     19.766  74.597  33.133  1.00 15.61    A   N
ATOM  1104  CA  LEU A 144     18.397  74.174  32.850  1.00 16.29    A   C
ATOM  1105  CB  LEU A 144     17.920  74.855  31.567  1.00 18.23    A   C
ATOM  1106  CG  LEU A 144     17.915  76.379  31.743  1.00 21.65    A   C
ATOM  1107  CD1 LEU A 144     17.543  77.079  30.440  1.00 21.02    A   C
ATOM  1108  CD2 LEU A 144     16.931  76.741  32.854  1.00 19.77    A   C
ATOM  1109  C   LEU A 144     18.171  72.657  32.772  1.00 15.16    A   C
ATOM  1110  O   LEU A 144     17.036  72.184  32.874  1.00 13.64    A   O
ATOM  1111  N   PHE A 145     19.238  71.888  32.600  1.00 13.93    A   N
ATOM  1112  CA  PHE A 145     19.080  70.437  32.545  1.00 11.95    A   C
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Figure 4U

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ATOM  1113  CB  PHE A 145      20.436  69.742  32.374  1.00 13.43      A   C
ATOM  1114  CG  PHE A 145      21.000  69.808  30.976  1.00 17.43      A   C
ATOM  1115  CD1 PHE A 145      22.248  69.260  30.703  1.00 15.45      A   C
ATOM  1116  CD2 PHE A 145      20.287  70.399  29.933  1.00 17.04      A   C
ATOM  1117  CE1 PHE A 145      22.783  69.295  29.420  1.00 18.35      A   C
ATOM  1118  CE2 PHE A 145      20.815  70.440  28.642  1.00 15.38      A   C
ATOM  1119  CZ  PHE A 145      22.064  69.889  28.385  1.00 16.89      A   C
ATOM  1120  C   PHE A 145      18.436  69.956  33.846  1.00 12.03      A   C
ATOM  1121  O   PHE A 145      17.600  69.064  33.839  1.00 11.95      A   O
ATOM  1122  N   VAL A 146      18.813  70.564  34.965  1.00 12.43      A   N
ATOM  1123  CA  VAL A 146      18.269  70.150  36.255  1.00 11.55      A   C
ATOM  1124  CB  VAL A 146      18.931  70.941  37.420  1.00 11.44      A   C
ATOM  1125  CG1 VAL A 146      18.203  70.669  38.739  1.00 12.27      A   C
ATOM  1126  CG2 VAL A 146      20.389  70.523  37.541  1.00 12.17      A   C
ATOM  1127  C   VAL A 146      16.741  70.243  36.344  1.00 13.17      A   C
ATOM  1128  O   VAL A 146      16.081  69.236  36.566  1.00 13.35      A   O
ATOM  1129  N   PRO A 147      16.157  71.442  36.168  1.00 14.55      A   N
ATOM  1130  CD  PRO A 147      16.725  72.794  36.014  1.00 12.51      A   C
ATOM  1131  CA  PRO A 147      14.693  71.491  36.260  1.00 15.45      A   C
ATOM  1132  CB  PRO A 147      14.386  72.995  36.197  1.00 16.91      A   C
ATOM  1133  CG  PRO A 147      15.556  73.569  35.463  1.00 13.21      A   C
ATOM  1134  C   PRO A 147      13.972  70.682  35.178  1.00 13.90      A   C
ATOM  1135  O   PRO A 147      12.910  70.111  35.433  1.00 15.62      A   O
ATOM  1136  N   LEU A 148      14.549  70.614  33.982  1.00 11.79      A   N
ATOM  1137  CA  LEU A 148      13.929  69.844  32.911  1.00 13.83      A   C
ATOM  1138  CB  LEU A 148      14.748  69.947  31.620  1.00 15.89      A   C
ATOM  1139  CG  LEU A 148      14.193  70.877  30.540  1.00 14.82      A   C
ATOM  1140  CD1 LEU A 148      14.146  72.296  31.057  1.00 18.80      A   C
ATOM  1141  CD2 LEU A 148      15.070  70.792  29.300  1.00 16.16      A   C
ATOM  1142  C   LEU A 148      13.833  68.389  33.336  1.00 13.84      A   C
ATOM  1143  O   LEU A 148      12.786  67.755  33.204  1.00 15.22      A   O
ATOM  1144  N   ILE A 149      14.935  67.872  33.861  1.00 12.81      A   N
ATOM  1145  CA  ILE A 149      14.985  66.493  34.312  1.00 13.21      A   C
ATOM  1146  CB  ILE A 149      16.425  66.111  34.703  1.00 14.51      A   C
ATOM  1147  CG2 ILE A 149      16.444  64.756  35.402  1.00 12.63      A   C
ATOM  1148  CG1 ILE A 149      17.291  66.093  33.434  1.00 15.10      A   C
ATOM  1149  CD1 ILE A 149      18.777  65.893  33.673  1.00 10.57      A   C
ATOM  1150  C   ILE A 149      14.026  66.258  35.470  1.00 14.45      A   C
ATOM  1151  O   ILE A 149      13.425  65.195  35.571  1.00 15.79      A   O
ATOM  1152  N   GLU A 150      13.859  67.256  36.328  1.00 14.06      A   N
ATOM  1153  CA  GLU A 150      12.943  67.121  37.449  1.00 15.01      A   C
ATOM  1154  CB  GLU A 150      13.206  68.228  38.466  1.00 18.77      A   C
ATOM  1155  CG  GLU A 150      14.447  67.930  39.291  1.00 26.06      A   C
ATOM  1156  CD  GLU A 150      14.824  69.044  40.227  1.00 28.16      A   C
ATOM  1157  OE1 GLU A 150      15.731  68.821  41.056  1.00 26.46      A   O
ATOM  1158  OE2 GLU A 150      14.222  70.138  40.128  1.00 31.52      A   O
ATOM  1159  C   GLU A 150      11.481  67.116  37.000  1.00 15.40      A   C
ATOM  1160  O   GLU A 150      10.615  66.617  37.719  1.00 14.17      A   O
ATOM  1161  N   GLU A 151      11.212  67.680  35.822  1.00 13.23      A   N
ATOM  1162  CA  GLU A 151       9.860  67.703  35.265  1.00 15.55      A   C
ATOM  1163  CB  GLU A 151       9.619  68.971  34.442  1.00 16.54      A   C
ATOM  1164  CG  GLU A 151       9.533  70.248  35.267  1.00 20.37      A   C
ATOM  1165  CD  GLU A 151       8.528  70.151  36.401  1.00 23.39      A   C
ATOM  1166  OE1 GLU A 151       7.332  69.901  36.134  1.00 24.54      A   O
ATOM  1167  OE2 GLU A 151       8.937  70.326  37.566  1.00 27.18      A   O
ATOM  1168  C   GLU A 151       9.687  66.487  34.368  1.00 17.22      A   C
ATOM  1169  O   GLU A 151       8.668  66.331  33.687  1.00 16.37      A   O
ATOM  1170  N   SER A 152      10.702  65.632  34.376  1.00 18.04      A   N
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Figure 4V

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ATOM  1171  CA  SER A 152      10.722  64.413  33.578  1.00 18.02      A   C
ATOM  1172  CB  SER A 152       9.559  63.493  33.949  1.00 19.94      A   C
ATOM  1173  OG  SER A 152       9.768  62.207  33.390  1.00 18.81      A   O
ATOM  1174  C   SER A 152      10.699  64.673  32.081  1.00 20.44      A   C
ATOM  1175  O   SER A 152      10.013  63.980  31.323  1.00 22.59      A   O
ATOM  1176  N   ILE A 153      11.443  65.682  31.653  1.00 19.73      A   N
ATOM  1177  CA  ILE A 153      11.541  65.998  30.239  1.00 21.13      A   C
ATOM  1178  CB  ILE A 153      11.541  67.521  30.016  1.00 23.26      A   C
ATOM  1179  CG2 ILE A 153      11.800  67.846  28.546  1.00 22.78      A   C
ATOM  1180  CG1 ILE A 153      10.190  68.086  30.474  1.00 25.17      A   C
ATOM  1181  CD1 ILE A 153      10.005  69.547  30.207  1.00 30.23      A   C
ATOM  1182  C   ILE A 153      12.865  65.372  29.832  1.00 21.67      A   C
ATOM  1183  O   ILE A 153      13.900  66.037  29.784  1.00 20.32      A   O
ATOM  1184  N   LEU A 154      12.811  64.069  29.565  1.00 18.75      A   N
ATOM  1185  CA  LEU A 154      13.986  63.281  29.218  1.00 20.85      A   C
ATOM  1186  CB  LEU A 154      13.939  61.972  30.003  1.00 21.22      A   C
ATOM  1187  CG  LEU A 154      13.540  62.197  31.467  1.00 22.53      A   C
ATOM  1188  CD1 LEU A 154      13.353  60.868  32.182  1.00 21.31      A   C
ATOM  1189  CD2 LEU A 154      14.604  63.040  32.154  1.00 20.71      A   C
ATOM  1190  C   LEU A 154      14.131  62.994  27.726  1.00 21.27      A   C
ATOM  1191  O   LEU A 154      14.969  62.194  27.313  1.00 20.75      A   O
ATOM  1192  N   GLU A 155      13.302  63.649  26.927  1.00 23.77      A   N
ATOM  1193  CA  GLU A 155      13.333  63.499  25.478  1.00 26.10      A   C
ATOM  1194  CB  GLU A 155      12.948  62.069  25.074  1.00 30.66      A   C
ATOM  1195  CG  GLU A 155      11.661  61.554  25.686  1.00 38.37      A   C
ATOM  1196  CD  GLU A 155      10.445  61.898  24.860  1.00 42.76      A   C
ATOM  1197  OE1 GLU A 155       9.322  61.571  25.299  1.00 48.12      A   O
ATOM  1198  OE2 GLU A 155      10.609  62.488  23.771  1.00 46.52      A   O
ATOM  1199  C   GLU A 155      12.366  64.517  24.893  1.00 24.72      A   C
ATOM  1200  O   GLU A 155      11.759  65.288  25.633  1.00 23.59      A   O
ATOM  1201  N   GLY A 156      12.236  64.538  23.573  1.00 23.02      A   N
ATOM  1202  CA  GLY A 156      11.333  65.492  22.958  1.00 21.08      A   C
ATOM  1203  C   GLY A 156      12.047  66.742  22.485  1.00 22.30      A   C
ATOM  1204  O   GLY A 156      13.243  66.925  22.728  1.00 21.15      A   O
ATOM  1205  N   GLU A 157      11.299  67.612  21.817  1.00 20.99      A   N
ATOM  1206  CA  GLU A 157      11.847  68.844  21.268  1.00 22.12      A   C
ATOM  1207  CB  GLU A 157      10.786  69.539  20.412  1.00 25.41      A   C
ATOM  1208  CG  GLU A 157      11.366  70.505  19.398  1.00 32.26      A   C
ATOM  1209  CD  GLU A 157      10.304  71.341  18.720  1.00 37.00      A   C
ATOM  1210  OE1 GLU A 157       9.332  70.758  18.186  1.00 41.42      A   O
ATOM  1211  OE2 GLU A 157      10.443  72.583  18.719  1.00 39.91      A   O
ATOM  1212  C   GLU A 157      12.386  69.835  22.302  1.00 19.65      A   C
ATOM  1213  O   GLU A 157      13.377  70.518  22.053  1.00 18.65      A   O
ATOM  1214  N   LEU A 158      11.734  69.925  23.453  1.00 18.49      A   N
ATOM  1215  CA  LEU A 158      12.172  70.861  24.485  1.00 20.02      A   C
ATOM  1216  CB  LEU A 158      11.174  70.870  25.653  1.00 19.53      A   C
ATOM  1217  CG  LEU A 158      11.410  71.891  26.773  1.00 21.01      A   C
ATOM  1218  CD1 LEU A 158      11.661  73.280  26.191  1.00 20.32      A   C
ATOM  1219  CD2 LEU A 158      10.197  71.910  27.697  1.00 19.63      A   C
ATOM  1220  C   LEU A 158      13.581  70.529  24.976  1.00 17.50      A   C
ATOM  1221  O   LEU A 158      14.424  71.417  25.101  1.00 17.99      A   O
ATOM  1222  N   LEU A 159      13.846  69.253  25.240  1.00 18.72      A   N
ATOM  1223  CA  LEU A 159      15.180  68.856  25.693  1.00 17.84      A   C
ATOM  1224  CB  LEU A 159      15.202  67.377  26.105  1.00 17.62      A   C
ATOM  1225  CG  LEU A 159      16.585  66.818  26.488  1.00 16.01      A   C
ATOM  1226  CD1 LEU A 159      17.125  67.557  27.713  1.00 16.76      A   C
ATOM  1227  CD2 LEU A 159      16.478  65.324  26.775  1.00 16.92      A   C
ATOM  1228  C   LEU A 159      16.185  69.091  24.571  1.00 18.06      A   C
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Figure 4W

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ATOM  1229  O   LEU A 159     17.274  69.629  24.792  1.00 15.90      A   O
ATOM  1230  N   GLU A 160     15.805  68.686  23.363  1.00 17.23      A   N
ATOM  1231  CA  GLU A 160     16.660  68.846  22.199  1.00 19.74      A   C
ATOM  1232  CB  GLU A 160     15.936  68.322  20.951  1.00 22.63      A   C
ATOM  1233  CG  GLU A 160     16.613  68.624  19.612  1.00 25.09      A   C
ATOM  1234  CD  GLU A 160     18.020  68.058  19.496  1.00 28.46      A   C
ATOM  1235  OE1 GLU A 160     18.320  67.041  20.156  1.00 24.99      A   O
ATOM  1236  OE2 GLU A 160     18.824  68.626  18.725  1.00 29.33      A   O
ATOM  1237  C   GLU A 160     17.025  70.316  22.023  1.00 17.75      A   C
ATOM  1238  O   GLU A 160     18.188  70.655  21.795  1.00 17.75      A   O
ATOM  1239  N   THR A 161     16.031  71.188  22.140  1.00 15.91      A   N
ATOM  1240  CA  THR A 161     16.274  72.615  21.984  1.00 17.08      A   C
ATOM  1241  CB  THR A 161     14.955  73.402  21.946  1.00 19.03      A   C
ATOM  1242  OG1 THR A 161     14.165  72.943  20.841  1.00 18.83      A   O
ATOM  1243  CG2 THR A 161     15.225  74.888  21.770  1.00 18.63      A   C
ATOM  1244  C   THR A 161     17.159  73.154  23.104  1.00 16.80      A   C
ATOM  1245  O   THR A 161     17.998  74.029  22.875  1.00 16.81      A   O
ATOM  1246  N   CYS A 162     16.977  72.623  24.309  1.00 15.47      A   N
ATOM  1247  CA  CYS A 162     17.772  73.054  25.451  1.00 16.48      A   C
ATOM  1248  CB  CYS A 162     17.217  72.456  26.748  1.00 17.44      A   C
ATOM  1249  SG  CYS A 162     17.994  73.125  28.246  1.00 17.16      A   S
ATOM  1250  C   CYS A 162     19.226  72.624  25.264  1.00 16.12      A   C
ATOM  1251  O   CYS A 162     20.148  73.390  25.547  1.00 15.64      A   O
ATOM  1252  N   MET A 163     19.433  71.395  24.797  1.00 16.12      A   N
ATOM  1253  CA  MET A 163     20.792  70.913  24.578  1.00 16.90      A   C
ATOM  1254  CB  MET A 163     20.796  69.446  24.152  1.00 17.54      A   C
ATOM  1255  CG  MET A 163     20.259  68.491  25.198  1.00 18.15      A   C
ATOM  1256  SD  MET A 163     20.679  66.775  24.864  1.00 18.78      A   S
ATOM  1257  CE  MET A 163     19.539  66.408  23.514  1.00 18.51      A   C
ATOM  1258  C   MET A 163     21.427  71.760  23.483  1.00 16.80      A   C
ATOM  1259  O   MET A 163     22.601  72.109  23.554  1.00 17.90      A   O
ATOM  1260  N   HIS A 164     20.637  72.083  22.467  1.00 17.35      A   N
ATOM  1261  CA  HIS A 164     21.119  72.893  21.359  1.00 18.77      A   C
ATOM  1262  CB  HIS A 164     20.009  73.065  20.317  1.00 21.03      A   C
ATOM  1263  CG  HIS A 164     20.451  73.784  19.082  1.00 26.61      A   C
ATOM  1264  CD2 HIS A 164     20.862  73.317  17.879  1.00 27.02      A   C
ATOM  1265  ND1 HIS A 164     20.559  75.156  19.018  1.00 26.82      A   N
ATOM  1266  CE1 HIS A 164     21.020  75.503  17.829  1.00 28.20      A   C
ATOM  1267  NE2 HIS A 164     21.212  74.406  17.119  1.00 26.69      A   N
ATOM  1268  C   HIS A 164     21.573  74.249  21.872  1.00 17.93      A   C
ATOM  1269  O   HIS A 164     22.630  74.758  21.483  1.00 18.32      A   O
ATOM  1270  N   TYR A 165     20.775  74.821  22.765  1.00 16.78      A   N
ATOM  1271  CA  TYR A 165     21.073  76.120  23.352  1.00 17.03      A   C
ATOM  1272  CB  TYR A 165     20.004  76.486  24.383  1.00 16.70      A   C
ATOM  1273  CG  TYR A 165     20.323  77.728  25.186  1.00 14.36      A   C
ATOM  1274  CD1 TYR A 165     20.249  78.998  24.611  1.00 18.03      A   C
ATOM  1275  CE1 TYR A 165     20.567  80.144  25.350  1.00 17.68      A   C
ATOM  1276  CD2 TYR A 165     20.722  77.633  26.518  1.00 15.98      A   C
ATOM  1277  CE2 TYR A 165     21.042  78.767  27.263  1.00 15.67      A   C
ATOM  1278  CZ  TYR A 165     20.964  80.015  26.675  1.00 17.67      A   C
ATOM  1279  OH  TYR A 165     21.296  81.128  27.414  1.00 19.35      A   O
ATOM  1280  C   TYR A 165     22.440  76.144  24.025  1.00 18.18      A   C
ATOM  1281  O   TYR A 165     23.202  77.089  23.848  1.00 18.56      A   O
ATOM  1282  N   TYR A 166     22.745  75.101  24.795  1.00 16.65      A   N
ATOM  1283  CA  TYR A 166     24.016  75.022  25.516  1.00 16.14      A   C
ATOM  1284  CB  TYR A 166     23.879  74.113  26.745  1.00 15.22      A   C
ATOM  1285  CG  TYR A 166     23.063  74.681  27.887  1.00 14.44      A   C
ATOM  1286  CD1 TYR A 166     21.955  73.994  28.380  1.00 13.39      A   C
```

Figure 4X

ATOM 1287 CE1 TYR A 166 21.202 74.506 29.438 1.00 14.31 A C
ATOM 1288 CD2 TYR A 166 23.403 75.898 28.481 1.00 14.07 A C
ATOM 1289 CE2 TYR A 166 22.660 76.419 29.537 1.00 13.27 A C
ATOM 1290 CZ TYR A 166 21.558 75.717 30.008 1.00 15.59 A C
ATOM 1291 OH TYR A 166 20.800 76.228 31.033 1.00 13.70 A O
ATOM 1292 C TYR A 166 25.207 74.520 24.710 1.00 16.15 A C
ATOM 1293 O TYR A 166 26.320 75.020 24.862 1.00 18.32 A O
ATOM 1294 N PHE A 167 24.977 73.532 23.858 1.00 16.40 A N
ATOM 1295 CA PHE A 167 26.063 72.926 23.099 1.00 19.32 A C
ATOM 1296 CB PHE A 167 25.696 71.466 22.811 1.00 18.55 A C
ATOM 1297 CG PHE A 167 25.487 70.633 24.056 1.00 17.57 A C
ATOM 1298 CD1 PHE A 167 24.611 69.551 24.044 1.00 17.73 A C
ATOM 1299 CD2 PHE A 167 26.179 70.920 25.232 1.00 17.53 A C
ATOM 1300 CE1 PHE A 167 24.429 68.766 25.186 1.00 17.59 A C
ATOM 1301 CE2 PHE A 167 26.005 70.140 26.378 1.00 15.09 A C
ATOM 1302 CZ PHE A 167 25.130 69.063 26.354 1.00 15.31 A C
ATOM 1303 C PHE A 167 26.517 73.613 21.810 1.00 21.91 A C
ATOM 1304 O PHE A 167 27.693 73.529 21.444 1.00 18.63 A O
ATOM 1305 N THR A 168 25.600 74.293 21.128 1.00 23.53 A N
ATOM 1306 CA THR A 168 25.940 74.958 19.871 1.00 25.11 A C
ATOM 1307 CB THR A 168 24.757 75.788 19.346 1.00 24.47 A C
ATOM 1308 OG1 THR A 168 23.646 74.919 19.099 1.00 28.03 A O
ATOM 1309 CG2 THR A 168 25.133 76.488 18.048 1.00 28.49 A C
ATOM 1310 C THR A 168 27.182 75.849 19.920 1.00 24.43 A C
ATOM 1311 O THR A 168 27.989 75.836 18.995 1.00 26.62 A O
ATOM 1312 N PRO A 169 27.347 76.640 20.992 1.00 25.87 A N
ATOM 1313 CD PRO A 169 26.337 76.983 22.009 1.00 23.89 A C
ATOM 1314 CA PRO A 169 28.512 77.523 21.113 1.00 28.42 A C
ATOM 1315 CB PRO A 169 28.198 78.329 22.372 1.00 25.95 A C
ATOM 1316 CG PRO A 169 26.709 78.406 22.351 1.00 26.22 A C
ATOM 1317 C PRO A 169 29.868 76.813 21.210 1.00 30.41 A C
ATOM 1318 O PRO A 169 30.914 77.440 21.035 1.00 30.45 A O
ATOM 1319 N LEU A 170 29.853 75.512 21.487 1.00 32.27 A N
ATOM 1320 CA LEU A 170 31.094 74.755 21.611 1.00 34.59 A C
ATOM 1321 CB LEU A 170 30.808 73.338 22.098 1.00 33.83 A C
ATOM 1322 CG LEU A 170 30.417 73.202 23.568 1.00 32.01 A C
ATOM 1323 CD1 LEU A 170 30.035 71.760 23.848 1.00 29.69 A C
ATOM 1324 CD2 LEU A 170 31.579 73.641 24.458 1.00 29.22 A C
ATOM 1325 C LEU A 170 31.897 74.677 20.323 1.00 37.74 A C
ATOM 1326 O LEU A 170 31.358 74.386 19.254 1.00 39.31 A O
ATOM 1327 N GLU A 171 33.197 74.924 20.434 1.00 40.03 A N
ATOM 1328 CA GLU A 171 34.076 74.871 19.276 1.00 43.34 A C
ATOM 1329 CB GLU A 171 34.750 76.229 19.067 1.00 48.27 A C
ATOM 1330 CG GLU A 171 33.759 77.349 18.782 1.00 54.56 A C
ATOM 1331 CD GLU A 171 33.072 77.200 17.431 1.00 59.45 A C
ATOM 1332 OE1 GLU A 171 32.919 76.051 16.953 1.00 60.27 A O
ATOM 1333 OE2 GLU A 171 32.672 78.237 16.852 1.00 61.77 A O
ATOM 1334 C GLU A 171 35.120 73.777 19.447 1.00 42.59 A C
ATOM 1335 O GLU A 171 36.239 73.888 18.951 1.00 43.77 A O
ATOM 1336 N ILE A 172 34.741 72.717 20.155 1.00 40.35 A N
ATOM 1337 CA ILE A 172 35.636 71.589 20.391 1.00 38.22 A C
ATOM 1338 CB ILE A 172 36.155 71.569 21.842 1.00 37.75 A C
ATOM 1339 CG2 ILE A 172 36.806 72.901 22.184 1.00 34.13 A C
ATOM 1340 CG1 ILE A 172 34.997 71.276 22.797 1.00 36.28 A C
ATOM 1341 CD1 ILE A 172 35.430 70.993 24.225 1.00 40.90 A C
ATOM 1342 C ILE A 172 34.911 70.272 20.145 1.00 36.42 A C
ATOM 1343 O ILE A 172 33.688 70.200 20.222 1.00 39.20 A O
ATOM 1344 N LEU A 173 35.674 69.231 19.838 1.00 34.80 A N

Figure 4Y

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ATOM  1345  CA  LEU A 173      35.104  67.910  19.612  1.00 32.15      A   C
ATOM  1346  CB  LEU A 173      35.718  67.265  18.363  1.00 33.04      A   C
ATOM  1347  CG  LEU A 173      35.480  67.998  17.037  1.00 34.61      A   C
ATOM  1348  CD1 LEU A 173      36.221  67.290  15.910  1.00 33.74      A   C
ATOM  1349  CD2 LEU A 173      33.979  68.056  16.747  1.00 34.77      A   C
ATOM  1350  C   LEU A 173      35.454  67.102  20.855  1.00 29.45      A   C
ATOM  1351  O   LEU A 173      36.481  66.424  20.896  1.00 27.62      A   O
ATOM  1352  N   PRO A 174      34.598  67.167  21.891  1.00 27.18      A   N
ATOM  1353  CD  PRO A 174      33.272  67.811  21.931  1.00 26.43      A   C
ATOM  1354  CA  PRO A 174      34.858  66.432  23.132  1.00 24.33      A   C
ATOM  1355  CB  PRO A 174      33.646  66.772  24.003  1.00 25.04      A   C
ATOM  1356  CG  PRO A 174      32.560  67.015  22.997  1.00 27.39      A   C
ATOM  1357  C   PRO A 174      35.067  64.934  22.991  1.00 21.39      A   C
ATOM  1358  O   PRO A 174      34.335  64.250  22.277  1.00 22.17      A   O
ATOM  1359  N   GLU A 175      36.088  64.438  23.679  1.00 19.42      A   N
ATOM  1360  CA  GLU A 175      36.405  63.021  23.683  1.00 19.85      A   C
ATOM  1361  CB  GLU A 175      37.905  62.821  23.465  1.00 21.90      A   C
ATOM  1362  CG  GLU A 175      38.320  62.869  21.999  1.00 27.70      A   C
ATOM  1363  CD  GLU A 175      39.823  62.943  21.802  1.00 27.64      A   C
ATOM  1364  OE1 GLU A 175      40.565  62.242  22.523  1.00 28.19      A   O
ATOM  1365  OE2 GLU A 175      40.260  63.701  20.913  1.00 30.42      A   O
ATOM  1366  C   GLU A 175      35.983  62.473  25.044  1.00 19.80      A   C
ATOM  1367  O   GLU A 175      35.855  61.263  25.239  1.00 19.75      A   O
ATOM  1368  N   VAL A 176      35.762  63.383  25.986  1.00 18.80      A   N
ATOM  1369  CA  VAL A 176      35.349  63.006  27.330  1.00 17.58      A   C
ATOM  1370  CB  VAL A 176      36.550  62.981  28.313  1.00 16.92      A   C
ATOM  1371  CG1 VAL A 176      36.091  62.488  29.676  1.00 15.99      A   C
ATOM  1372  CG2 VAL A 176      37.661  62.087  27.772  1.00 16.67      A   C
ATOM  1373  C   VAL A 176      34.330  64.014  27.840  1.00 16.96      A   C
ATOM  1374  O   VAL A 176      34.533  65.224  27.746  1.00 17.95      A   O
ATOM  1375  N   ILE A 177      33.222  63.509  28.362  1.00 17.35      A   N
ATOM  1376  CA  ILE A 177      32.184  64.373  28.902  1.00 15.36      A   C
ATOM  1377  CB  ILE A 177      30.873  64.272  28.100  1.00 15.94      A   C
ATOM  1378  CG2 ILE A 177      29.805  65.149  28.759  1.00 14.07      A   C
ATOM  1379  CG1 ILE A 177      31.113  64.699  26.647  1.00 17.19      A   C
ATOM  1380  CD1 ILE A 177      29.880  64.597  25.748  1.00 18.12      A   C
ATOM  1381  C   ILE A 177      31.896  63.970  30.334  1.00 14.25      A   C
ATOM  1382  O   ILE A 177      31.499  62.833  30.609  1.00 15.75      A   O
ATOM  1383  N   ILE A 178      32.108  64.900  31.253  1.00 14.90      A   N
ATOM  1384  CA  ILE A 178      31.841  64.618  32.647  1.00 12.36      A   C
ATOM  1385  CB  ILE A 178      32.770  65.419  33.573  1.00 14.08      A   C
ATOM  1386  CG2 ILE A 178      32.465  65.085  35.026  1.00 10.97      A   C
ATOM  1387  CG1 ILE A 178      34.229  65.095  33.248  1.00 13.91      A   C
ATOM  1388  CD1 ILE A 178      35.235  65.846  34.106  1.00 13.08      A   C
ATOM  1389  C   ILE A 178      30.396  64.988  32.950  1.00 12.88      A   C
ATOM  1390  O   ILE A 178      29.949  66.103  32.671  1.00 13.50      A   O
ATOM  1391  N   LEU A 179      29.659  64.038  33.506  1.00 12.90      A   N
ATOM  1392  CA  LEU A 179      28.270  64.288  33.867  1.00 14.35      A   C
ATOM  1393  CB  LEU A 179      27.465  62.992  33.717  1.00 14.31      A   C
ATOM  1394  CG  LEU A 179      27.542  62.418  32.298  1.00 15.12      A   C
ATOM  1395  CD1 LEU A 179      26.919  61.033  32.251  1.00 20.10      A   C
ATOM  1396  CD2 LEU A 179      26.844  63.361  31.336  1.00 20.25      A   C
ATOM  1397  C   LEU A 179      28.320  64.760  35.319  1.00 13.67      A   C
ATOM  1398  O   LEU A 179      27.829  64.085  36.224  1.00 15.54      A   O
ATOM  1399  N   GLY A 180      28.930  65.931  35.512  1.00 11.65      A   N
ATOM  1400  CA  GLY A 180      29.117  66.517  36.834  1.00 12.90      A   C
ATOM  1401  C   GLY A 180      27.910  67.040  37.593  1.00 10.74      A   C
ATOM  1402  O   GLY A 180      27.955  68.116  38.191  1.00 12.43      A   O
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Figure 4Z

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ATOM  1403  N   CYS A 181     26.835  66.267  37.589  1.00 11.19      A   N
ATOM  1404  CA  CYS A 181     25.608  66.640  38.287  1.00 12.85      A   C
ATOM  1405  CB  CYS A 181     24.832  67.662  37.455  1.00 10.63      A   C
ATOM  1406  SG  CYS A 181     23.232  68.156  38.139  1.00 12.80      A   S
ATOM  1407  C   CYS A 181     24.769  65.379  38.482  1.00 10.40      A   C
ATOM  1408  O   CYS A 181     24.655  64.567  37.565  1.00 12.33      A   O
ATOM  1409  N   THR A 182     24.195  65.218  39.673  1.00 11.84      A   N
ATOM  1410  CA  THR A 182     23.374  64.050  39.993  1.00 10.35      A   C
ATOM  1411  CB  THR A 182     22.661  64.207  41.363  1.00 10.67      A   C
ATOM  1412  OG1 THR A 182     21.912  65.435  41.381  1.00  8.58      A   O
ATOM  1413  CG2 THR A 182     23.672  64.197  42.500  1.00  7.64      A   C
ATOM  1414  C   THR A 182     22.283  63.760  38.966  1.00 11.06      A   C
ATOM  1415  O   THR A 182     21.936  62.610  38.733  1.00 10.76      A   O
ATOM  1416  N   HIS A 183     21.739  64.810  38.364  1.00  9.82      A   N
ATOM  1417  CA  HIS A 183     20.649  64.666  37.400  1.00 12.23      A   C
ATOM  1418  CB  HIS A 183     19.884  65.990  37.276  1.00 10.20      A   C
ATOM  1419  CG  HIS A 183     19.136  66.386  38.510  1.00 10.97      A   C
ATOM  1420  CD2 HIS A 183     17.905  66.930  38.668  1.00  7.50      A   C
ATOM  1421  ND1 HIS A 183     19.677  66.290  39.774  1.00 11.77      A   N
ATOM  1422  CE1 HIS A 183     18.812  66.758  40.658  1.00 10.61      A   C
ATOM  1423  NE2 HIS A 183     17.729  67.154  40.012  1.00 10.59      A   N
ATOM  1424  C   HIS A 183     21.020  64.221  35.990  1.00 10.73      A   C
ATOM  1425  O   HIS A 183     20.228  63.569  35.323  1.00 12.38      A   O
ATOM  1426  N   PHE A 184     22.221  64.570  35.545  1.00 12.86      A   N
ATOM  1427  CA  PHE A 184     22.645  64.280  34.180  1.00 12.13      A   C
ATOM  1428  CB  PHE A 184     23.988  64.976  33.925  1.00 11.91      A   C
ATOM  1429  CG  PHE A 184     23.927  66.488  34.096  1.00 11.77      A   C
ATOM  1430  CD1 PHE A 184     25.057  67.276  33.896  1.00 13.67      A   C
ATOM  1431  CD2 PHE A 184     22.739  67.116  34.482  1.00  9.45      A   C
ATOM  1432  CE1 PHE A 184     25.009  68.666  34.081  1.00 11.33      A   C
ATOM  1433  CE2 PHE A 184     22.681  68.502  34.670  1.00 12.83      A   C
ATOM  1434  CZ  PHE A 184     23.819  69.278  34.469  1.00  9.95      A   C
ATOM  1435  C   PHE A 184     22.655  62.833  33.670  1.00 12.53      A   C
ATOM  1436  O   PHE A 184     22.429  62.596  32.481  1.00 14.09      A   O
ATOM  1437  N   PRO A 185     22.902  61.847  34.545  1.00 13.81      A   N
ATOM  1438  CD  PRO A 185     23.442  61.881  35.918  1.00 14.48      A   C
ATOM  1439  CA  PRO A 185     22.893  60.475  34.026  1.00 13.96      A   C
ATOM  1440  CB  PRO A 185     23.165  59.640  35.275  1.00 14.58      A   C
ATOM  1441  CG  PRO A 185     24.112  60.522  36.032  1.00 12.13      A   C
ATOM  1442  C   PRO A 185     21.554  60.121  33.367  1.00 15.04      A   C
ATOM  1443  O   PRO A 185     21.492  59.261  32.489  1.00 13.75      A   O
ATOM  1444  N   LEU A 186     20.485  60.790  33.791  1.00 13.98      A   N
ATOM  1445  CA  LEU A 186     19.156  60.525  33.243  1.00 13.19      A   C
ATOM  1446  CB  LEU A 186     18.080  61.193  34.108  1.00 13.71      A   C
ATOM  1447  CG  LEU A 186     17.634  60.379  35.334  1.00 15.55      A   C
ATOM  1448  CD1 LEU A 186     18.802  60.174  36.288  1.00 18.92      A   C
ATOM  1449  CD2 LEU A 186     16.493  61.099  36.027  1.00 14.26      A   C
ATOM  1450  C   LEU A 186     18.982  60.931  31.778  1.00 14.41      A   C
ATOM  1451  O   LEU A 186     18.010  60.533  31.137  1.00 14.59      A   O
ATOM  1452  N   ILE A 187     19.905  61.734  31.255  1.00 14.30      A   N
ATOM  1453  CA  ILE A 187     19.854  62.140  29.849  1.00 14.33      A   C
ATOM  1454  CB  ILE A 187     19.485  63.633  29.667  1.00 13.17      A   C
ATOM  1455  CG2 ILE A 187     18.052  63.871  30.096  1.00 11.03      A   C
ATOM  1456  CG1 ILE A 187     20.446  64.523  30.453  1.00 12.17      A   C
ATOM  1457  CD1 ILE A 187     20.256  66.011  30.170  1.00 14.07      A   C
ATOM  1458  C   ILE A 187     21.197  61.890  29.168  1.00 14.64      A   C
ATOM  1459  O   ILE A 187     21.487  62.447  28.108  1.00 13.68      A   O
ATOM  1460  N   ALA A 188     22.008  61.035  29.781  1.00 15.37      A   N
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Figure 4AA

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ATOM  1461  CA  ALA A 188      23.322  60.707  29.243  1.00 16.86      A   C
ATOM  1462  CB  ALA A 188      23.965  59.607  30.075  1.00 15.17      A   C
ATOM  1463  C   ALA A 188      23.244  60.280  27.776  1.00 17.17      A   C
ATOM  1464  O   ALA A 188      23.979  60.797  26.938  1.00 15.74      A   O
ATOM  1465  N   GLN A 189      22.353  59.340  27.470  1.00 17.32      A   N
ATOM  1466  CA  GLN A 189      22.203  58.857  26.101  1.00 18.82      A   C
ATOM  1467  CB  GLN A 189      21.162  57.741  26.050  1.00 23.61      A   C
ATOM  1468  CG  GLN A 189      21.199  56.919  24.774  1.00 30.80      A   C
ATOM  1469  CD  GLN A 189      22.592  56.391  24.458  1.00 36.03      A   C
ATOM  1470  OE1 GLN A 189      23.321  55.942  25.347  1.00 36.39      A   O
ATOM  1471  NE2 GLN A 189      22.965  56.435  23.184  1.00 38.93      A   N
ATOM  1472  C   GLN A 189      21.794  59.995  25.169  1.00 17.49      A   C
ATOM  1473  O   GLN A 189      22.280  60.092  24.041  1.00 17.22      A   O
ATOM  1474  N   LYS A 190      20.894  60.851  25.639  1.00 17.64      A   N
ATOM  1475  CA  LYS A 190      20.449  61.986  24.841  1.00 16.93      A   C
ATOM  1476  CB  LYS A 190      19.338  62.750  25.565  1.00 17.51      A   C
ATOM  1477  CG  LYS A 190      17.998  62.038  25.578  1.00 21.98      A   C
ATOM  1478  CD  LYS A 190      17.462  61.852  24.166  1.00 25.56      A   C
ATOM  1479  CE  LYS A 190      16.064  61.256  24.188  1.00 30.02      A   C
ATOM  1480  NZ  LYS A 190      15.428  61.242  22.839  1.00 32.59      A   N
ATOM  1481  C   LYS A 190      21.624  62.919  24.572  1.00 17.12      A   C
ATOM  1482  O   LYS A 190      21.755  63.468  23.481  1.00 19.51      A   O
ATOM  1483  N   ILE A 191      22.483  63.097  25.570  1.00 15.92      A   N
ATOM  1484  CA  ILE A 191      23.643  63.963  25.413  1.00 15.53      A   C
ATOM  1485  CB  ILE A 191      24.348  64.194  26.769  1.00 16.74      A   C
ATOM  1486  CG2 ILE A 191      25.698  64.877  26.558  1.00 17.54      A   C
ATOM  1487  CG1 ILE A 191      23.447  65.048  27.668  1.00 16.67      A   C
ATOM  1488  CD1 ILE A 191      24.051  65.372  29.014  1.00 17.95      A   C
ATOM  1489  C   ILE A 191      24.615  63.350  24.413  1.00 17.26      A   C
ATOM  1490  O   ILE A 191      25.099  64.027  23.508  1.00 16.51      A   O
ATOM  1491  N   GLU A 192      24.892  62.062  24.566  1.00 17.44      A   N
ATOM  1492  CA  GLU A 192      25.792  61.387  23.643  1.00 18.42      A   C
ATOM  1493  CB  GLU A 192      25.937  59.909  24.007  1.00 20.11      A   C
ATOM  1494  CG  GLU A 192      26.885  59.159  23.085  1.00 26.76      A   C
ATOM  1495  CD  GLU A 192      26.872  57.665  23.322  1.00 32.66      A   C
ATOM  1496  OE1 GLU A 192      25.884  57.005  22.936  1.00 37.07      A   O
ATOM  1497  OE2 GLU A 192      27.846  57.152  23.906  1.00 37.14      A   O
ATOM  1498  C   GLU A 192      25.209  61.499  22.241  1.00 17.46      A   C
ATOM  1499  O   GLU A 192      25.912  61.804  21.283  1.00 15.49      A   O
ATOM  1500  N   GLY A 193      23.910  61.249  22.136  1.00 19.60      A   N
ATOM  1501  CA  GLY A 193      23.247  61.319  20.851  1.00 18.22      A   C
ATOM  1502  C   GLY A 193      23.344  62.683  20.199  1.00 20.98      A   C
ATOM  1503  O   GLY A 193      23.518  62.781  18.983  1.00 19.02      A   O
ATOM  1504  N   TYR A 194      23.230  63.742  20.997  1.00 19.99      A   N
ATOM  1505  CA  TYR A 194      23.302  65.087  20.450  1.00 19.30      A   C
ATOM  1506  CB  TYR A 194      23.081  66.136  21.545  1.00 21.79      A   C
ATOM  1507  CG  TYR A 194      23.038  67.544  20.997  1.00 22.73      A   C
ATOM  1508  CD1 TYR A 194      21.822  68.170  20.713  1.00 25.33      A   C
ATOM  1509  CE1 TYR A 194      21.784  69.442  20.133  1.00 26.15      A   C
ATOM  1510  CD2 TYR A 194      24.216  68.226  20.692  1.00 24.23      A   C
ATOM  1511  CE2 TYR A 194      24.190  69.493  20.109  1.00 23.26      A   C
ATOM  1512  CZ  TYR A 194      22.973  70.092  19.830  1.00 25.26      A   C
ATOM  1513  OH  TYR A 194      22.941  71.327  19.222  1.00 28.86      A   O
ATOM  1514  C   TYR A 194      24.660  65.313  19.788  1.00 20.71      A   C
ATOM  1515  O   TYR A 194      24.738  65.782  18.653  1.00 18.94      A   O
ATOM  1516  N   PHE A 195      25.732  64.980  20.496  1.00 19.26      A   N
ATOM  1517  CA  PHE A 195      27.062  65.169  19.942  1.00 21.38      A   C
ATOM  1518  CB  PHE A 195      28.126  64.952  21.020  1.00 20.73      A   C
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Figure 4BB

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ATOM  1519  CG  PHE A 195     28.251  66.103  21.971  1.00 20.61      A   C
ATOM  1520  CD1 PHE A 195     27.488  66.158  23.131  1.00 19.23      A   C
ATOM  1521  CD2 PHE A 195     29.097  67.165  21.673  1.00 21.43      A   C
ATOM  1522  CE1 PHE A 195     27.565  67.263  23.986  1.00 20.28      A   C
ATOM  1523  CE2 PHE A 195     29.183  68.273  22.515  1.00 18.52      A   C
ATOM  1524  CZ  PHE A 195     28.416  68.323  23.673  1.00 19.62      A   C
ATOM  1525  C   PHE A 195     27.352  64.290  18.730  1.00 21.31      A   C
ATOM  1526  O   PHE A 195     28.045  64.713  17.806  1.00 21.45      A   O
ATOM  1527  N   MET A 196     26.822  63.072  18.720  1.00 22.22      A   N
ATOM  1528  CA  MET A 196     27.059  62.190  17.584  1.00 24.31      A   C
ATOM  1529  CB  MET A 196     26.655  60.749  17.915  1.00 25.67      A   C
ATOM  1530  CG  MET A 196     27.528  60.084  18.971  1.00 26.49      A   C
ATOM  1531  SD  MET A 196     29.295  60.205  18.575  1.00 30.70      A   S
ATOM  1532  CE  MET A 196     29.481  58.865  17.401  1.00 31.02      A   C
ATOM  1533  C   MET A 196     26.293  62.667  16.354  1.00 25.42      A   C
ATOM  1534  O   MET A 196     26.734  62.451  15.227  1.00 23.73      A   O
ATOM  1535  N   GLY A 197     25.157  63.328  16.571  1.00 25.90      A   N
ATOM  1536  CA  GLY A 197     24.361  63.805  15.451  1.00 26.44      A   C
ATOM  1537  C   GLY A 197     24.566  65.258  15.054  1.00 29.06      A   C
ATOM  1538  O   GLY A 197     24.129  65.681  13.981  1.00 30.51      A   O
ATOM  1539  N   HIS A 198     25.233  66.030  15.903  1.00 27.75      A   N
ATOM  1540  CA  HIS A 198     25.456  67.441  15.612  1.00 28.55      A   C
ATOM  1541  CB  HIS A 198     24.824  68.293  16.705  1.00 28.88      A   C
ATOM  1542  CG  HIS A 198     23.330  68.234  16.718  1.00 26.12      A   C
ATOM  1543  CD2 HIS A 198     22.470  67.535  17.495  1.00 26.28      A   C
ATOM  1544  ND1 HIS A 198     22.553  68.943  15.828  1.00 27.58      A   N
ATOM  1545  CE1 HIS A 198     21.277  68.687  16.060  1.00 27.01      A   C
ATOM  1546  NE2 HIS A 198     21.200  67.835  17.066  1.00 26.83      A   N
ATOM  1547  C   HIS A 198     26.923  67.792  15.457  1.00 30.79      A   C
ATOM  1548  O   HIS A 198     27.270  68.941  15.180  1.00 32.29      A   O
ATOM  1549  N   PHE A 199     27.785  66.800  15.644  1.00 30.80      A   N
ATOM  1550  CA  PHE A 199     29.220  66.999  15.498  1.00 33.66      A   C
ATOM  1551  CB  PHE A 199     29.906  67.052  16.866  1.00 35.46      A   C
ATOM  1552  CG  PHE A 199     29.565  68.275  17.676  1.00 39.04      A   C
ATOM  1553  CD1 PHE A 199     28.281  68.463  18.182  1.00 39.24      A   C
ATOM  1554  CD2 PHE A 199     30.537  69.237  17.945  1.00 40.88      A   C
ATOM  1555  CE1 PHE A 199     27.968  69.591  18.944  1.00 40.57      A   C
ATOM  1556  CE2 PHE A 199     30.236  70.370  18.707  1.00 42.99      A   C
ATOM  1557  CZ  PHE A 199     28.948  70.547  19.207  1.00 40.25      A   C
ATOM  1558  C   PHE A 199     29.790  65.855  14.673  1.00 32.87      A   C
ATOM  1559  O   PHE A 199     29.170  64.798  14.547  1.00 32.00      A   O
ATOM  1560  N   ALA A 200     30.972  66.064  14.108  1.00 34.09      A   N
ATOM  1561  CA  ALA A 200     31.605  65.040  13.288  1.00 34.34      A   C
ATOM  1562  CB  ALA A 200     32.381  65.690  12.154  1.00 35.22      A   C
ATOM  1563  C   ALA A 200     32.532  64.168  14.119  1.00 34.93      A   C
ATOM  1564  O   ALA A 200     33.704  63.996  13.782  1.00 35.08      A   O
ATOM  1565  N   LEU A 201     32.012  63.618  15.209  1.00 34.85      A   N
ATOM  1566  CA  LEU A 201     32.821  62.765  16.067  1.00 34.78      A   C
ATOM  1567  CB  LEU A 201     32.210  62.690  17.472  1.00 35.79      A   C
ATOM  1568  CG  LEU A 201     32.120  64.015  18.231  1.00 35.31      A   C
ATOM  1569  CD1 LEU A 201     31.513  63.760  19.603  1.00 35.13      A   C
ATOM  1570  CD2 LEU A 201     33.498  64.641  18.365  1.00 35.35      A   C
ATOM  1571  C   LEU A 201     32.906  61.366  15.462  1.00 34.07      A   C
ATOM  1572  O   LEU A 201     31.887  60.773  15.104  1.00 35.38      A   O
ATOM  1573  N   PRO A 202     34.128  60.817  15.344  1.00 33.66      A   N
ATOM  1574  CD  PRO A 202     35.409  61.457  15.698  1.00 32.39      A   C
ATOM  1575  CA  PRO A 202     34.353  59.475  14.779  1.00 32.85      A   C
ATOM  1576  CB  PRO A 202     35.872  59.404  14.655  1.00 33.65      A   C
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Figure 4CC

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ATOM  1577  CG  PRO A 202      36.343  60.272  15.793  1.00 34.48      A   C
ATOM  1578  C   PRO A 202      33.790  58.355  15.649  1.00 33.17      A   C
ATOM  1579  O   PRO A 202      33.402  57.297  15.151  1.00 30.49      A   O
ATOM  1580  N   THR A 203      33.773  58.599  16.956  1.00 31.52      A   N
ATOM  1581  CA  THR A 203      33.248  57.634  17.919  1.00 31.65      A   C
ATOM  1582  CB  THR A 203      34.338  56.676  18.426  1.00 32.68      A   C
ATOM  1583  OG1 THR A 203      35.425  57.424  18.979  1.00 35.29      A   O
ATOM  1584  CG2 THR A 203      34.828  55.781  17.302  1.00 37.32      A   C
ATOM  1585  C   THR A 203      32.688  58.386  19.117  1.00 30.86      A   C
ATOM  1586  O   THR A 203      33.168  59.451  19.461  1.00 27.18      A   O
ATOM  1587  N   PRO A 204      31.671  57.817  19.775  1.00 29.89      A   N
ATOM  1588  CD  PRO A 204      31.126  56.473  19.492  1.00 29.77      A   C
ATOM  1589  CA  PRO A 204      31.061  58.463  20.945  1.00 28.24      A   C
ATOM  1590  CB  PRO A 204      30.047  57.449  21.462  1.00 29.94      A   C
ATOM  1591  CG  PRO A 204      30.111  56.276  20.568  1.00 30.77      A   C
ATOM  1592  C   PRO A 204      32.096  58.803  22.007  1.00 25.79      A   C
ATOM  1593  O   PRO A 204      33.032  58.041  22.269  1.00 25.89      A   O
ATOM  1594  N   PRO A 205      31.961  59.981  22.626  1.00 23.44      A   N
ATOM  1595  CD  PRO A 205      30.990  61.063  22.358  1.00 24.13      A   C
ATOM  1596  CA  PRO A 205      32.915  60.378  23.670  1.00 22.08      A   C
ATOM  1597  CB  PRO A 205      32.600  61.852  23.873  1.00 24.52      A   C
ATOM  1598  CG  PRO A 205      31.125  61.932  23.587  1.00 24.69      A   C
ATOM  1599  C   PRO A 205      32.705  59.546  24.927  1.00 19.36      A   C
ATOM  1600  O   PRO A 205      31.637  58.961  25.125  1.00 18.49      A   O
ATOM  1601  N   LEU A 206      33.722  59.492  25.776  1.00 18.43      A   N
ATOM  1602  CA  LEU A 206      33.626  58.762  27.037  1.00 18.50      A   C
ATOM  1603  CB  LEU A 206      35.018  58.513  27.619  1.00 20.51      A   C
ATOM  1604  CG  LEU A 206      35.095  57.847  28.996  1.00 22.39      A   C
ATOM  1605  CD1 LEU A 206      34.491  56.439  28.946  1.00 22.36      A   C
ATOM  1606  CD2 LEU A 206      36.552  57.791  29.435  1.00 24.60      A   C
ATOM  1607  C   LEU A 206      32.822  59.615  28.017  1.00 18.04      A   C
ATOM  1608  O   LEU A 206      33.163  60.770  28.253  1.00 16.95      A   O
ATOM  1609  N   LEU A 207      31.746  59.049  28.554  1.00 16.00      A   N
ATOM  1610  CA  LEU A 207      30.909  59.748  29.521  1.00 17.26      A   C
ATOM  1611  CB  LEU A 207      29.433  59.412  29.304  1.00 18.06      A   C
ATOM  1612  CG  LEU A 207      28.664  60.071  28.158  1.00 24.42      A   C
ATOM  1613  CD1 LEU A 207      29.448  59.984  26.863  1.00 25.51      A   C
ATOM  1614  CD2 LEU A 207      27.310  59.373  28.012  1.00 24.48      A   C
ATOM  1615  C   LEU A 207      31.318  59.314  30.922  1.00 16.98      A   C
ATOM  1616  O   LEU A 207      31.388  58.120  31.215  1.00 18.46      A   O
ATOM  1617  N   ILE A 208      31.592  60.276  31.792  1.00 13.50      A   N
ATOM  1618  CA  ILE A 208      31.983  59.940  33.150  1.00 14.98      A   C
ATOM  1619  CB  ILE A 208      33.112  60.864  33.659  1.00 16.20      A   C
ATOM  1620  CG2 ILE A 208      33.468  60.509  35.101  1.00 16.97      A   C
ATOM  1621  CG1 ILE A 208      34.345  60.722  32.763  1.00 16.39      A   C
ATOM  1622  CD1 ILE A 208      34.984  59.333  32.784  1.00 17.91      A   C
ATOM  1623  C   ILE A 208      30.771  60.069  34.057  1.00 15.79      A   C
ATOM  1624  O   ILE A 208      30.193  61.150  34.194  1.00 15.47      A   O
ATOM  1625  N   HIS A 209      30.390  58.951  34.669  1.00 15.02      A   N
ATOM  1626  CA  HIS A 209      29.238  58.895  35.567  1.00 14.90      A   C
ATOM  1627  CB  HIS A 209      28.502  57.569  35.333  1.00 17.49      A   C
ATOM  1628  CG  HIS A 209      27.271  57.387  36.169  1.00 19.71      A   C
ATOM  1629  CD2 HIS A 209      27.116  57.192  37.500  1.00 20.19      A   C
ATOM  1630  ND1 HIS A 209      26.004  57.336  35.625  1.00 21.72      A   N
ATOM  1631  CE1 HIS A 209      25.123  57.114  36.584  1.00 17.63      A   C
ATOM  1632  NE2 HIS A 209      25.772  57.023  37.732  1.00 22.48      A   N
ATOM  1633  C   HIS A 209      29.744  59.006  37.011  1.00 13.24      A   C
ATOM  1634  O   HIS A 209      30.546  58.191  37.458  1.00 13.01      A   O
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Figure 4DD

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ATOM   1635  N   SER A 210      29.275  60.018  37.734  1.00 12.05      A   N
ATOM   1636  CA  SER A 210      29.709  60.238  39.109  1.00 11.23      A   C
ATOM   1637  CB  SER A 210      28.977  61.442  39.701  1.00 11.83      A   C
ATOM   1638  OG  SER A 210      29.140  62.587  38.881  1.00 12.14      A   O
ATOM   1639  C   SER A 210      29.529  59.031  40.032  1.00 12.17      A   C
ATOM   1640  O   SER A 210      30.370  58.774  40.890  1.00 11.45      A   O
ATOM   1641  N   GLY A 211      28.432  58.303  39.861  1.00 13.88      A   N
ATOM   1642  CA  GLY A 211      28.178  57.142  40.698  1.00 15.08      A   C
ATOM   1643  C   GLY A 211      29.147  56.004  40.446  1.00 16.38      A   C
ATOM   1644  O   GLY A 211      29.744  55.461  41.378  1.00 15.04      A   O
ATOM   1645  N   ASP A 212      29.311  55.630  39.183  1.00 15.98      A   N
ATOM   1646  CA  ASP A 212      30.231  54.552  38.860  1.00 16.82      A   C
ATOM   1647  CB  ASP A 212      30.208  54.264  37.365  1.00 19.63      A   C
ATOM   1648  CG  ASP A 212      28.847  53.798  36.895  1.00 23.61      A   C
ATOM   1649  OD1 ASP A 212      28.145  53.131  37.692  1.00 25.34      A   O
ATOM   1650  OD2 ASP A 212      28.486  54.086  35.738  1.00 21.50      A   O
ATOM   1651  C   ASP A 212      31.638  54.917  39.303  1.00 16.04      A   C
ATOM   1652  O   ASP A 212      32.375  54.073  39.807  1.00 15.40      A   O
ATOM   1653  N   ALA A 213      31.994  56.185  39.135  1.00 12.67      A   N
ATOM   1654  CA  ALA A 213      33.317  56.667  39.517  1.00 14.11      A   C
ATOM   1655  CB  ALA A 213      33.493  58.126  39.076  1.00 11.29      A   C
ATOM   1656  C   ALA A 213      33.560  56.540  41.022  1.00 12.53      A   C
ATOM   1657  O   ALA A 213      34.607  56.049  41.452  1.00 13.00      A   O
ATOM   1658  N   ILE A 214      32.603  56.973  41.834  1.00 13.61      A   N
ATOM   1659  CA  ILE A 214      32.808  56.875  43.271  1.00 11.94      A   C
ATOM   1660  CB  ILE A 214      31.748  57.701  44.065  1.00 12.63      A   C
ATOM   1661  CG2 ILE A 214      30.367  57.085  43.938  1.00 15.04      A   C
ATOM   1662  CG1 ILE A 214      32.174  57.795  45.530  1.00 12.30      A   C
ATOM   1663  CD1 ILE A 214      31.429  58.832  46.317  1.00 11.04      A   C
ATOM   1664  C   ILE A 214      32.855  55.405  43.719  1.00 13.71      A   C
ATOM   1665  O   ILE A 214      33.595  55.061  44.643  1.00 12.81      A   O
ATOM   1666  N   VAL A 215      32.096  54.538  43.053  1.00 13.33      A   N
ATOM   1667  CA  VAL A 215      32.118  53.109  43.387  1.00 13.18      A   C
ATOM   1668  CB  VAL A 215      31.165  52.293  42.474  1.00 13.68      A   C
ATOM   1669  CG1 VAL A 215      31.481  50.792  42.579  1.00 14.80      A   C
ATOM   1670  CG2 VAL A 215      29.707  52.537  42.876  1.00 10.93      A   C
ATOM   1671  C   VAL A 215      33.550  52.599  43.190  1.00 15.07      A   C
ATOM   1672  O   VAL A 215      34.115  51.933  44.065  1.00 12.73      A   O
ATOM   1673  N   GLU A 216      34.136  52.924  42.039  1.00 13.86      A   N
ATOM   1674  CA  GLU A 216      35.503  52.511  41.738  1.00 17.89      A   C
ATOM   1675  CB  GLU A 216      35.973  53.120  40.414  1.00 21.27      A   C
ATOM   1676  CG  GLU A 216      35.112  52.807  39.204  1.00 27.92      A   C
ATOM   1677  CD  GLU A 216      35.637  53.492  37.941  1.00 34.02      A   C
ATOM   1678  OE1 GLU A 216      36.824  53.286  37.609  1.00 31.93      A   O
ATOM   1679  OE2 GLU A 216      34.868  54.236  37.285  1.00 35.33      A   O
ATOM   1680  C   GLU A 216      36.447  52.971  42.846  1.00 17.32      A   C
ATOM   1681  O   GLU A 216      37.245  52.188  43.363  1.00 16.80      A   O
ATOM   1682  N   TYR A 217      36.352  54.248  43.204  1.00 16.20      A   N
ATOM   1683  CA  TYR A 217      37.200  54.818  44.244  1.00 16.23      A   C
ATOM   1684  CB  TYR A 217      36.900  56.308  44.432  1.00 14.73      A   C
ATOM   1685  CG  TYR A 217      37.693  56.942  45.557  1.00 17.55      A   C
ATOM   1686  CD1 TYR A 217      39.053  57.202  45.418  1.00 18.17      A   C
ATOM   1687  CE1 TYR A 217      39.797  57.738  46.475  1.00 18.51      A   C
ATOM   1688  CD2 TYR A 217      37.089  57.234  46.780  1.00 16.61      A   C
ATOM   1689  CE2 TYR A 217      37.815  57.765  47.836  1.00 17.74      A   C
ATOM   1690  CZ  TYR A 217      39.168  58.014  47.680  1.00 19.47      A   C
ATOM   1691  OH  TYR A 217      39.891  58.526  48.735  1.00 18.42      A   O
ATOM   1692  C   TYR A 217      37.041  54.116  45.584  1.00 16.31      A   C
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Figure 4EE

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ATOM  1693  O   TYR A 217     38.028  53.715  46.199  1.00 16.78    A   O
ATOM  1694  N   LEU A 218     35.798  53.995  46.045  1.00 15.56    A   N
ATOM  1695  CA  LEU A 218     35.509  53.353  47.324  1.00 18.16    A   C
ATOM  1696  CB  LEU A 218     33.993  53.344  47.575  1.00 15.21    A   C
ATOM  1697  CG  LEU A 218     33.321  54.705  47.799  1.00 15.27    A   C
ATOM  1698  CD1 LEU A 218     31.798  54.546  47.756  1.00 14.34    A   C
ATOM  1699  CD2 LEU A 218     33.775  55.294  49.129  1.00 13.25    A   C
ATOM  1700  C   LEU A 218     36.058  51.926  47.402  1.00 18.45    A   C
ATOM  1701  O   LEU A 218     36.648  51.531  48.409  1.00 18.06    A   O
ATOM  1702  N   GLN A 219     35.871  51.150  46.341  1.00 17.77    A   N
ATOM  1703  CA  GLN A 219     36.367  49.778  46.335  1.00 19.66    A   C
ATOM  1704  CB  GLN A 219     36.042  49.097  45.005  1.00 18.42    A   C
ATOM  1705  CG  GLN A 219     34.577  49.147  44.645  1.00 17.80    A   C
ATOM  1706  CD  GLN A 219     34.282  48.496  43.318  1.00 17.89    A   C
ATOM  1707  OE1 GLN A 219     35.071  48.596  42.372  1.00 18.96    A   O
ATOM  1708  NE2 GLN A 219     33.134  47.837  43.228  1.00 13.87    A   N
ATOM  1709  C   GLN A 219     37.876  49.740  46.567  1.00 19.63    A   C
ATOM  1710  O   GLN A 219     38.368  48.964  47.380  1.00 19.95    A   O
ATOM  1711  N   GLN A 220     38.605  50.593  45.859  1.00 21.16    A   N
ATOM  1712  CA  GLN A 220     40.057  50.621  45.992  1.00 24.11    A   C
ATOM  1713  CB  GLN A 220     40.681  51.372  44.811  1.00 25.85    A   C
ATOM  1714  CG  GLN A 220     42.197  51.445  44.885  1.00 34.94    A   C
ATOM  1715  CD  GLN A 220     42.830  51.975  43.615  1.00 40.03    A   C
ATOM  1716  OE1 GLN A 220     44.050  52.152  43.548  1.00 44.37    A   O
ATOM  1717  NE2 GLN A 220     42.010  52.227  42.598  1.00 41.95    A   N
ATOM  1718  C   GLN A 220     40.534  51.242  47.304  1.00 22.63    A   C
ATOM  1719  O   GLN A 220     41.275  50.617  48.062  1.00 21.00    A   O
ATOM  1720  N   LYS A 221     40.104  52.472  47.564  1.00 21.71    A   N
ATOM  1721  CA  LYS A 221     40.503  53.194  48.770  1.00 22.37    A   C
ATOM  1722  CB  LYS A 221     39.830  54.570  48.795  1.00 21.53    A   C
ATOM  1723  CG  LYS A 221     39.984  55.325  50.111  1.00 25.31    A   C
ATOM  1724  CD  LYS A 221     41.443  55.615  50.439  1.00 26.19    A   C
ATOM  1725  CE  LYS A 221     41.579  56.244  51.818  1.00 29.00    A   C
ATOM  1726  NZ  LYS A 221     42.999  56.511  52.159  1.00 29.71    A   N
ATOM  1727  C   LYS A 221     40.221  52.464  50.084  1.00 22.42    A   C
ATOM  1728  O   LYS A 221     41.090  52.376  50.953  1.00 21.37    A   O
ATOM  1729  N   TYR A 222     39.005  51.950  50.229  1.00 20.94    A   N
ATOM  1730  CA  TYR A 222     38.616  51.250  51.442  1.00 21.75    A   C
ATOM  1731  CB  TYR A 222     37.251  51.762  51.903  1.00 22.02    A   C
ATOM  1732  CG  TYR A 222     37.277  53.247  52.204  1.00 20.42    A   C
ATOM  1733  CD1 TYR A 222     36.737  54.178  51.314  1.00 18.91    A   C
ATOM  1734  CE1 TYR A 222     36.866  55.549  51.545  1.00 20.88    A   C
ATOM  1735  CD2 TYR A 222     37.938  53.725  53.336  1.00 21.77    A   C
ATOM  1736  CE2 TYR A 222     38.074  55.080  53.577  1.00 19.97    A   C
ATOM  1737  CZ  TYR A 222     37.540  55.988  52.679  1.00 20.71    A   C
ATOM  1738  OH  TYR A 222     37.705  57.330  52.909  1.00 16.95    A   O
ATOM  1739  C   TYR A 222     38.637  49.731  51.350  1.00 21.67    A   C
ATOM  1740  O   TYR A 222     38.112  49.040  52.226  1.00 20.83    A   O
ATOM  1741  N   ALA A 223     39.264  49.219  50.292  1.00 21.20    A   N
ATOM  1742  CA  ALA A 223     39.408  47.774  50.077  1.00 22.92    A   C
ATOM  1743  CB  ALA A 223     40.466  47.204  50.984  1.00 23.23    A   C
ATOM  1744  C   ALA A 223     38.105  47.055  50.330  1.00 23.19    A   C
ATOM  1745  O   ALA A 223     38.024  46.162  51.180  1.00 20.95    A   O
ATOM  1746  N   LEU A 224     37.088  47.426  49.565  1.00 25.19    A   N
ATOM  1747  CA  LEU A 224     35.759  46.839  49.692  1.00 24.53    A   C
ATOM  1748  CB  LEU A 224     34.703  47.937  49.609  1.00 22.99    A   C
ATOM  1749  CG  LEU A 224     34.869  49.090  50.607  1.00 21.68    A   C
ATOM  1750  CD1 LEU A 224     33.731  50.099  50.443  1.00 22.66    A   C
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Figure 4FF

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ATOM  1751 CD2 LEU A 224     34.875 48.531 52.022 1.00 23.83    A   C
ATOM  1752 C  LEU A 224     35.576 45.852 48.551 1.00 24.10    A   C
ATOM  1753 O  LEU A 224     35.569 46.259 47.400 1.00 22.11    A   O
ATOM  1754 N  LYS A 225     35.368 44.572 48.866 1.00 26.47    A   N
ATOM  1755 CA  LYS A 225     35.212 43.532 47.846 1.00 25.75    A   C
ATOM  1756 CB  LYS A 225     35.880 42.233 48.331 1.00 26.74    A   C
ATOM  1757 CG  LYS A 225     37.358 42.380 48.669 1.00 28.32    A   C
ATOM  1758 CD  LYS A 225     38.185 42.652 47.421 1.00 31.42    A   C
ATOM  1759 CE  LYS A 225     38.157 41.461 46.478 1.00 32.69    A   C
ATOM  1760 NZ  LYS A 225     39.003 41.698 45.284 1.00 34.46    A   N
ATOM  1761 C  LYS A 225     33.803 43.213 47.340 1.00 24.95    A   C
ATOM  1762 O  LYS A 225     33.568 42.125 46.819 1.00 29.54    A   O
ATOM  1763 N  ASN A 226     32.870 44.143 47.489 1.00 23.13    A   N
ATOM  1764 CA  ASN A 226     31.498 43.938 47.019 1.00 20.01    A   C
ATOM  1765 CB  ASN A 226     31.469 43.729 45.500 1.00 19.42    A   C
ATOM  1766 CG  ASN A 226     32.287 44.755 44.751 1.00 23.12    A   C
ATOM  1767 OD1 ASN A 226     33.342 44.439 44.190 1.00 20.38    A   O
ATOM  1768 ND2 ASN A 226     31.814 45.995 44.743 1.00 16.65    A   N
ATOM  1769 C  ASN A 226     30.800 42.740 47.662 1.00 21.21    A   C
ATOM  1770 O  ASN A 226     30.086 41.999 46.981 1.00 18.29    A   O
ATOM  1771 N  ASN A 227     30.984 42.551 48.963 1.00 22.29    A   N
ATOM  1772 CA  ASN A 227     30.362 41.421 49.641 1.00 22.96    A   C
ATOM  1773 CB  ASN A 227     31.438 40.462 50.163 1.00 22.46    A   C
ATOM  1774 CG  ASN A 227     32.503 41.165 50.982 1.00 21.07    A   C
ATOM  1775 OD1 ASN A 227     32.223 42.137 51.679 1.00 19.99    A   O
ATOM  1776 ND2 ASN A 227     33.733 40.659 50.916 1.00 19.44    A   N
ATOM  1777 C  ASN A 227     29.428 41.805 50.783 1.00 24.57    A   C
ATOM  1778 O  ASN A 227     29.198 41.005 51.690 1.00 21.91    A   O
ATOM  1779 N  ALA A 228     28.891 43.021 50.741 1.00 23.23    A   N
ATOM  1780 CA  ALA A 228     27.969 43.481 51.776 1.00 26.14    A   C
ATOM  1781 CB  ALA A 228     27.806 45.001 51.699 1.00 22.82    A   C
ATOM  1782 C  ALA A 228     26.611 42.793 51.596 1.00 26.93    A   C
ATOM  1783 O  ALA A 228     26.405 42.077 50.619 1.00 26.75    A   O
ATOM  1784 N  CYS A 229     25.698 43.016 52.541 1.00 29.94    A   N
ATOM  1785 CA  CYS A 229     24.359 42.425 52.508 1.00 34.05    A   C
ATOM  1786 CB  CYS A 229     23.438 43.143 53.508 1.00 36.45    A   C
ATOM  1787 SG  CYS A 229     23.886 42.897 55.243 1.00 48.21    A   S
ATOM  1788 C  CYS A 229     23.730 42.476 51.124 1.00 35.31    A   C
ATOM  1789 O  CYS A 229     23.882 43.451 50.399 1.00 35.27    A   O
ATOM  1790 N  THR A 230     23.030 41.412 50.757 1.00 38.04    A   N
ATOM  1791 CA  THR A 230     22.378 41.380 49.466 1.00 40.97    A   C
ATOM  1792 CB  THR A 230     21.965 39.958 49.076 1.00 42.40    A   C
ATOM  1793 OG1 THR A 230     21.273 39.335 50.163 1.00 45.09    A   O
ATOM  1794 CG2 THR A 230     23.190 39.148 48.730 1.00 43.15    A   C
ATOM  1795 C  THR A 230     21.150 42.269 49.476 1.00 41.97    A   C
ATOM  1796 O  THR A 230     20.887 42.971 48.493 1.00 42.37    A   O
ATOM  1797 N  PHE A 231     20.376 42.232 50.552 1.00 42.74    A   N
ATOM  1798 CA  PHE A 231     19.230 43.108 50.576 1.00 43.96    A   C
ATOM  1799 CB  PHE A 231     17.938 42.321 50.366 1.00 49.35    A   C
ATOM  1800 CG  PHE A 231     17.721 41.990 48.907 1.00 55.66    A   C
ATOM  1801 CD1 PHE A 231     18.494 41.004 48.306 1.00 58.70    A   C
ATOM  1802 CD2 PHE A 231     16.903 42.785 48.088 1.00 58.59    A   C
ATOM  1803 CE1 PHE A 231     18.483 40.801 46.922 1.00 60.69    A   C
ATOM  1804 CE2 PHE A 231     16.879 42.597 46.701 1.00 60.58    A   C
ATOM  1805 CZ  PHE A 231     17.668 41.604 46.113 1.00 60.92    A   C
ATOM  1806 C  PHE A 231     19.335 43.912 51.838 1.00 40.83    A   C
ATOM  1807 O  PHE A 231     18.811 43.567 52.886 1.00 42.69    A   O
ATOM  1808 N  PRO A 232     20.153 44.975 51.722 1.00 35.76    A   N
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Figure 4GG

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ATOM  1809 CD  PRO A 232     20.672  45.196  50.347  1.00 35.27    A   C
ATOM  1810 CA  PRO A 232     20.579  46.028  52.651  1.00 32.93    A   C
ATOM  1811 CB  PRO A 232     21.689  46.764  51.874  1.00 32.41    A   C
ATOM  1812 CG  PRO A 232     21.363  46.497  50.424  1.00 32.47    A   C
ATOM  1813 C   PRO A 232     19.457  46.929  53.137  1.00 29.06    A   C
ATOM  1814 O   PRO A 232     18.456  47.146  52.452  1.00 27.86    A   O
ATOM  1815 N   LYS A 233     19.630  47.440  54.346  1.00 27.89    A   N
ATOM  1816 CA  LYS A 233     18.645  48.314  54.943  1.00 25.66    A   C
ATOM  1817 CB  LYS A 233     18.682  48.188  56.464  1.00 29.61    A   C
ATOM  1818 CG  LYS A 233     18.178  46.843  56.973  1.00 34.08    A   C
ATOM  1819 CD  LYS A 233     18.086  46.829  58.491  1.00 40.01    A   C
ATOM  1820 CE  LYS A 233     19.454  46.996  59.139  1.00 41.92    A   C
ATOM  1821 NZ  LYS A 233     19.351  47.038  60.626  1.00 44.78    A   N
ATOM  1822 C   LYS A 233     18.945  49.739  54.524  1.00 23.25    A   C
ATOM  1823 O   LYS A 233     20.042  50.248  54.738  1.00 20.72    A   O
ATOM  1824 N   VAL A 234     17.959  50.374  53.909  1.00 21.94    A   N
ATOM  1825 CA  VAL A 234     18.122  51.742  53.457  1.00 18.96    A   C
ATOM  1826 CB  VAL A 234     18.171  51.809  51.927  1.00 18.07    A   C
ATOM  1827 CG1 VAL A 234     18.407  53.242  51.484  1.00 15.91    A   C
ATOM  1828 CG2 VAL A 234     19.265  50.884  51.403  1.00 19.03    A   C
ATOM  1829 C   VAL A 234     16.982  52.622  53.945  1.00 19.45    A   C
ATOM  1830 O   VAL A 234     15.810  52.291  53.775  1.00 18.84    A   O
ATOM  1831 N   GLU A 235     17.332  53.749  54.550  1.00 18.70    A   N
ATOM  1832 CA  GLU A 235     16.333  54.682  55.044  1.00 19.65    A   C
ATOM  1833 CB  GLU A 235     16.584  55.029  56.513  1.00 20.87    A   C
ATOM  1834 CG  GLU A 235     16.619  53.849  57.461  1.00 24.25    A   C
ATOM  1835 CD  GLU A 235     16.762  54.287  58.908  1.00 26.71    A   C
ATOM  1836 OE1 GLU A 235     16.924  53.412  59.782  1.00 30.95    A   O
ATOM  1837 OE2 GLU A 235     16.710  55.509  59.174  1.00 28.58    A   O
ATOM  1838 C   GLU A 235     16.433  55.957  54.226  1.00 19.63    A   C
ATOM  1839 O   GLU A 235     17.522  56.339  53.793  1.00 19.08    A   O
ATOM  1840 N   PHE A 236     15.295  56.608  54.008  1.00 16.22    A   N
ATOM  1841 CA  PHE A 236     15.281  57.850  53.260  1.00 15.50    A   C
ATOM  1842 CB  PHE A 236     14.454  57.703  51.985  1.00 16.22    A   C
ATOM  1843 CG  PHE A 236     15.028  56.712  51.008  1.00 16.49    A   C
ATOM  1844 CD1 PHE A 236     14.734  55.352  51.117  1.00 14.80    A   C
ATOM  1845 CD2 PHE A 236     15.906  57.131  50.011  1.00 16.20    A   C
ATOM  1846 CE1 PHE A 236     15.311  54.423  50.249  1.00 16.35    A   C
ATOM  1847 CE2 PHE A 236     16.488  56.213  49.140  1.00 16.85    A   C
ATOM  1848 CZ  PHE A 236     16.191  54.857  49.258  1.00 18.08    A   C
ATOM  1849 C   PHE A 236     14.725  58.953  54.150  1.00 17.81    A   C
ATOM  1850 O   PHE A 236     13.669  58.808  54.771  1.00 17.48    A   O
ATOM  1851 N   HIS A 237     15.473  60.043  54.238  1.00 14.01    A   N
ATOM  1852 CA  HIS A 237     15.077  61.178  55.050  1.00 13.85    A   C
ATOM  1853 CB  HIS A 237     15.976  61.261  56.282  1.00 16.76    A   C
ATOM  1854 CG  HIS A 237     15.871  60.068  57.183  1.00 20.30    A   C
ATOM  1855 CD2 HIS A 237     16.529  58.884  57.176  1.00 22.69    A   C
ATOM  1856 ND1 HIS A 237     14.963  59.994  58.216  1.00 21.64    A   N
ATOM  1857 CE1 HIS A 237     15.065  58.816  58.808  1.00 24.58    A   C
ATOM  1858 NE2 HIS A 237     16.008  58.123  58.196  1.00 24.02    A   N
ATOM  1859 C   HIS A 237     15.240  62.421  54.190  1.00 12.98    A   C
ATOM  1860 O   HIS A 237     15.960  62.402  53.199  1.00 14.24    A   O
ATOM  1861 N   ALA A 238     14.573  63.500  54.571  1.00 14.25    A   N
ATOM  1862 CA  ALA A 238     14.656  64.745  53.822  1.00 14.74    A   C
ATOM  1863 CB  ALA A 238     13.867  64.622  52.523  1.00 13.87    A   C
ATOM  1864 C   ALA A 238     14.105  65.889  54.662  1.00 16.80    A   C
ATOM  1865 O   ALA A 238     13.416  65.662  55.659  1.00 13.41    A   O
ATOM  1866 N   SER A 239     14.419  67.118  54.265  1.00 16.83    A   N
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Figure 4HH

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ATOM   1867  CA  SER A 239      13.934  68.289  54.982  1.00 15.86      A   C
ATOM   1868  CB  SER A 239      14.874  69.472  54.749  1.00 17.78      A   C
ATOM   1869  OG  SER A 239      15.235  69.570  53.382  1.00 15.31      A   O
ATOM   1870  C   SER A 239      12.526  68.628  54.501  1.00 18.27      A   C
ATOM   1871  O   SER A 239      11.851  69.475  55.081  1.00 19.09      A   O
ATOM   1872  N   GLY A 240      12.093  67.950  53.440  1.00 19.12      A   N
ATOM   1873  CA  GLY A 240      10.764  68.172  52.891  1.00 18.85      A   C
ATOM   1874  C   GLY A 240      10.400  67.108  51.872  1.00 20.08      A   C
ATOM   1875  O   GLY A 240      11.262  66.321  51.462  1.00 19.84      A   O
ATOM   1876  N   ASP A 241       9.134  67.065  51.464  1.00 17.58      A   N
ATOM   1877  CA  ASP A 241       8.692  66.077  50.481  1.00 19.46      A   C
ATOM   1878  CB  ASP A 241       9.150  66.501  49.083  1.00 21.27      A   C
ATOM   1879  CG  ASP A 241       8.429  67.738  48.587  1.00 23.85      A   C
ATOM   1880  OD1 ASP A 241       7.247  67.610  48.206  1.00 26.32      A   O
ATOM   1881  OD2 ASP A 241       9.038  68.833  48.591  1.00 21.42      A   O
ATOM   1882  C   ASP A 241       9.257  64.694  50.803  1.00 16.99      A   C
ATOM   1883  O   ASP A 241       9.731  63.987  49.913  1.00 17.49      A   O
ATOM   1884  N   VAL A 242       9.208  64.316  52.076  1.00 15.93      A   N
ATOM   1885  CA  VAL A 242       9.737  63.025  52.516  1.00 14.13      A   C
ATOM   1886  CB  VAL A 242       9.894  62.990  54.052  1.00 17.19      A   C
ATOM   1887  CG1 VAL A 242      10.671  61.740  54.469  1.00 16.23      A   C
ATOM   1888  CG2 VAL A 242      10.612  64.248  54.523  1.00 18.97      A   C
ATOM   1889  C   VAL A 242       8.849  61.864  52.082  1.00 15.60      A   C
ATOM   1890  O   VAL A 242       9.341  60.808  51.660  1.00 12.78      A   O
ATOM   1891  N   ILE A 243       7.540  62.057  52.209  1.00 14.41      A   N
ATOM   1892  CA  ILE A 243       6.577  61.045  51.803  1.00 16.25      A   C
ATOM   1893  CB  ILE A 243       5.125  61.549  52.007  1.00 18.10      A   C
ATOM   1894  CG2 ILE A 243       4.123  60.554  51.414  1.00 20.99      A   C
ATOM   1895  CG1 ILE A 243       4.858  61.747  53.502  1.00 21.18      A   C
ATOM   1896  CD1 ILE A 243       3.485  62.293  53.817  1.00 20.78      A   C
ATOM   1897  C   ILE A 243       6.833  60.787  50.324  1.00 15.05      A   C
ATOM   1898  O   ILE A 243       6.885  59.639  49.878  1.00 16.76      A   O
ATOM   1899  N   TRP A 244       7.005  61.868  49.569  1.00 13.24      A   N
ATOM   1900  CA  TRP A 244       7.270  61.768  48.142  1.00 15.52      A   C
ATOM   1901  CB  TRP A 244       7.343  63.164  47.523  1.00 13.47      A   C
ATOM   1902  CG  TRP A 244       7.510  63.151  46.036  1.00 18.87      A   C
ATOM   1903  CD2 TRP A 244       8.732  63.342  45.312  1.00 17.48      A   C
ATOM   1904  CE2 TRP A 244       8.426  63.232  43.940  1.00 18.22      A   C
ATOM   1905  CE3 TRP A 244      10.057  63.594  45.693  1.00 17.59      A   C
ATOM   1906  CD1 TRP A 244       6.538  62.938  45.099  1.00 18.15      A   C
ATOM   1907  NE1 TRP A 244       7.083  62.988  43.835  1.00 18.29      A   N
ATOM   1908  CZ2 TRP A 244       9.399  63.366  42.943  1.00 20.22      A   C
ATOM   1909  CZ3 TRP A 244      11.024  63.727  44.702  1.00 18.36      A   C
ATOM   1910  CH2 TRP A 244      10.688  63.611  43.342  1.00 18.43      A   C
ATOM   1911  C   TRP A 244       8.590  61.042  47.891  1.00 14.64      A   C
ATOM   1912  O   TRP A 244       8.670  60.149  47.044  1.00 16.51      A   O
ATOM   1913  N   LEU A 245       9.628  61.436  48.623  1.00 13.56      A   N
ATOM   1914  CA  LEU A 245      10.941  60.814  48.459  1.00 12.19      A   C
ATOM   1915  CB  LEU A 245      11.946  61.416  49.444  1.00 11.28      A   C
ATOM   1916  CG  LEU A 245      13.379  60.875  49.342  1.00 11.24      A   C
ATOM   1917  CD1 LEU A 245      13.988  61.289  48.009  1.00 11.74      A   C
ATOM   1918  CD2 LEU A 245      14.223  61.407  50.490  1.00 10.22      A   C
ATOM   1919  C   LEU A 245      10.862  59.301  48.661  1.00 14.05      A   C
ATOM   1920  O   LEU A 245      11.439  58.537  47.884  1.00 12.33      A   O
ATOM   1921  N   GLU A 246      10.144  58.870  49.698  1.00 14.68      A   N
ATOM   1922  CA  GLU A 246      10.000  57.441  49.980  1.00 16.30      A   C
ATOM   1923  CB  GLU A 246       9.198  57.213  51.267  1.00 16.70      A   C
ATOM   1924  CG  GLU A 246       9.938  57.637  52.521  1.00 23.08      A   C
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Figure 4II

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ATOM  1925  CD  GLU A 246      9.544  56.818  53.737  1.00 25.63      A   C
ATOM  1926  OE1 GLU A 246      8.335  56.577  53.927  1.00 24.93      A   O
ATOM  1927  OE2 GLU A 246     10.444  56.423  54.508  1.00 27.10      A   O
ATOM  1928  C   GLU A 246      9.324  56.714  48.828  1.00 15.72      A   C
ATOM  1929  O   GLU A 246      9.691  55.589  48.494  1.00 15.40      A   O
ATOM  1930  N   ARG A 247      8.326  57.359  48.235  1.00 16.57      A   N
ATOM  1931  CA  ARG A 247      7.611  56.790  47.105  1.00 18.74      A   C
ATOM  1932  CB  ARG A 247      6.445  57.710  46.711  1.00 23.10      A   C
ATOM  1933  CG  ARG A 247      5.875  57.451  45.325  1.00 32.32      A   C
ATOM  1934  CD  ARG A 247      4.561  58.204  45.114  1.00 40.32      A   C
ATOM  1935  NE  ARG A 247      4.084  58.117  43.733  1.00 47.44      A   N
ATOM  1936  CZ  ARG A 247      4.569  58.835  42.722  1.00 49.78      A   C
ATOM  1937  NH1 ARG A 247      5.548  59.705  42.931  1.00 51.70      A   N
ATOM  1938  NH2 ARG A 247      4.079  58.682  41.497  1.00 52.43      A   N
ATOM  1939  C   ARG A 247      8.594  56.630  45.941  1.00 17.54      A   C
ATOM  1940  O   ARG A 247      8.654  55.578  45.299  1.00 14.31      A   O
ATOM  1941  N   GLN A 248      9.375  57.672  45.677  1.00 15.93      A   N
ATOM  1942  CA  GLN A 248     10.350  57.608  44.598  1.00 16.24      A   C
ATOM  1943  CB  GLN A 248     11.120  58.929  44.485  1.00 17.33      A   C
ATOM  1944  CG  GLN A 248     10.267  60.119  44.047  1.00 16.22      A   C
ATOM  1945  CD  GLN A 248      9.552  59.879  42.725  1.00 22.44      A   C
ATOM  1946  OE1 GLN A 248     10.184  59.627  41.694  1.00 22.85      A   O
ATOM  1947  NE2 GLN A 248      8.225  59.958  42.749  1.00 24.90      A   N
ATOM  1948  C   GLN A 248     11.324  56.453  44.815  1.00 15.90      A   C
ATOM  1949  O   GLN A 248     11.705  55.768  43.866  1.00 16.87      A   O
ATOM  1950  N   ALA A 249     11.720  56.231  46.065  1.00 15.92      A   N
ATOM  1951  CA  ALA A 249     12.644  55.146  46.384  1.00 15.55      A   C
ATOM  1952  CB  ALA A 249     13.015  55.191  47.857  1.00 16.80      A   C
ATOM  1953  C   ALA A 249     12.032  53.789  46.041  1.00 16.47      A   C
ATOM  1954  O   ALA A 249     12.685  52.943  45.426  1.00 16.21      A   O
ATOM  1955  N   LYS A 250     10.779  53.582  46.438  1.00 16.38      A   N
ATOM  1956  CA  LYS A 250     10.102  52.316  46.159  1.00 18.81      A   C
ATOM  1957  CB  LYS A 250      8.750  52.258  46.880  1.00 20.86      A   C
ATOM  1958  CG  LYS A 250      8.843  52.132  48.394  1.00 26.84      A   C
ATOM  1959  CD  LYS A 250      7.488  51.745  48.988  1.00 31.08      A   C
ATOM  1960  CE  LYS A 250      7.554  51.607  50.507  1.00 31.43      A   C
ATOM  1961  NZ  LYS A 250      7.896  52.899  51.156  1.00 29.87      A   N
ATOM  1962  C   LYS A 250      9.884  52.121  44.661  1.00 18.41      A   C
ATOM  1963  O   LYS A 250     10.073  51.024  44.125  1.00 15.17      A   O
ATOM  1964  N   GLU A 251      9.493  53.200  43.992  1.00 15.62      A   N
ATOM  1965  CA  GLU A 251      9.224  53.167  42.562  1.00 18.32      A   C
ATOM  1966  CB  GLU A 251      8.586  54.486  42.119  1.00 20.33      A   C
ATOM  1967  CG  GLU A 251      7.205  54.758  42.692  1.00 23.48      A   C
ATOM  1968  CD  GLU A 251      6.106  54.036  41.936  1.00 25.23      A   C
ATOM  1969  OE1 GLU A 251      6.415  53.361  40.932  1.00 28.49      A   O
ATOM  1970  OE2 GLU A 251      4.932  54.152  42.341  1.00 25.47      A   O
ATOM  1971  C   GLU A 251     10.448  52.921  41.694  1.00 20.06      A   C
ATOM  1972  O   GLU A 251     10.398  52.121  40.763  1.00 17.23      A   O
ATOM  1973  N   TRP A 252     11.547  53.606  41.997  1.00 19.52      A   N
ATOM  1974  CA  TRP A 252     12.748  53.489  41.175  1.00 20.14      A   C
ATOM  1975  CB  TRP A 252     13.276  54.885  40.832  1.00 18.05      A   C
ATOM  1976  CG  TRP A 252     12.305  55.710  40.043  1.00 18.22      A   C
ATOM  1977  CD2 TRP A 252     12.039  55.607  38.640  1.00 20.57      A   C
ATOM  1978  CE2 TRP A 252     11.017  56.533  38.339  1.00 20.85      A   C
ATOM  1979  CE3 TRP A 252     12.564  54.818  37.607  1.00 21.87      A   C
ATOM  1980  CD1 TRP A 252     11.460  56.669  40.523  1.00 17.88      A   C
ATOM  1981  NE1 TRP A 252     10.683  57.168  39.508  1.00 17.77      A   N
ATOM  1982  CZ2 TRP A 252     10.506  56.697  37.041  1.00 22.03      A   C
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Figure 4JJ

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ATOM  1983 CZ3 TRP A 252     12.055  54.978  36.314  1.00 21.57    A   C
ATOM  1984 CH2 TRP A 252     11.036  55.913  36.045  1.00 22.86    A   C
ATOM  1985 C   TRP A 252     13.902  52.641  41.688  1.00 22.39    A   C
ATOM  1986 O   TRP A 252     14.680  52.122  40.886  1.00 23.72    A   O
ATOM  1987 N   LEU A 253     14.024  52.504  43.003  1.00 22.18    A   N
ATOM  1988 CA  LEU A 253     15.106  51.717  43.588  1.00 25.35    A   C
ATOM  1989 CB  LEU A 253     15.809  52.524  44.680  1.00 20.44    A   C
ATOM  1990 CG  LEU A 253     16.355  53.904  44.285  1.00 21.92    A   C
ATOM  1991 CD1 LEU A 253     16.785  54.649  45.532  1.00 18.63    A   C
ATOM  1992 CD2 LEU A 253     17.530  53.758  43.316  1.00 20.79    A   C
ATOM  1993 C   LEU A 253     14.583  50.401  44.168  1.00 29.73    A   C
ATOM  1994 O   LEU A 253     15.357  49.570  44.647  1.00 31.04    A   O
ATOM  1995 N   LYS A 254     13.267  50.219  44.121  1.00 33.91    A   N
ATOM  1996 CA  LYS A 254     12.638  49.007  44.631  1.00 39.79    A   C
ATOM  1997 CB  LYS A 254     13.102  47.795  43.812  1.00 43.18    A   C
ATOM  1998 CG  LYS A 254     12.330  46.518  44.102  1.00 51.27    A   C
ATOM  1999 CD  LYS A 254     12.747  45.377  43.181  1.00 56.67    A   C
ATOM  2000 CE  LYS A 254     11.928  44.121  43.464  1.00 59.29    A   C
ATOM  2001 NZ  LYS A 254     10.463  44.368  43.307  1.00 62.20    A   N
ATOM  2002 C   LYS A 254     12.967  48.805  46.110  1.00 41.24    A   C
ATOM  2003 O   LYS A 254     13.111  47.678  46.586  1.00 42.02    A   O
ATOM  2004 N   LEU A 255     13.091  49.911  46.834  1.00 42.21    A   N
ATOM  2005 CA  LEU A 255     13.396  49.856  48.255  1.00 43.88    A   C
ATOM  2006 CB  LEU A 255     14.643  50.687  48.560  1.00 41.85    A   C
ATOM  2007 CG  LEU A 255     15.934  50.186  47.910  1.00 40.40    A   C
ATOM  2008 CD1 LEU A 255     17.065  51.143  48.229  1.00 40.11    A   C
ATOM  2009 CD2 LEU A 255     16.258  48.788  48.412  1.00 39.40    A   C
ATOM  2010 C   LEU A 255     12.211  50.365  49.070  1.00 46.21    A   C
ATOM  2011 O   LEU A 255     12.350  51.427  49.715  1.00 47.30    A   O
ATOM  2012 OXT LEU A 255     11.152  49.696  49.044  1.00 48.09    A   O
ATOM  2013 CB  MET B   1      3.272 103.508  55.905  1.00 23.27    B   C
ATOM  2014 CG  MET B   1      3.026 102.116  56.484  1.00 25.31    B   C
ATOM  2015 SD  MET B   1      1.613 101.253  55.747  1.00 29.32    B   S
ATOM  2016 CE  MET B   1      0.239 102.076  56.594  1.00 27.48    B   C
ATOM  2017 C   MET B   1      5.739 103.357  56.203  1.00 22.82    B   C
ATOM  2018 O   MET B   1      6.391 103.503  55.166  1.00 21.44    B   O
ATOM  2019 N   MET B   1      4.661 105.565  55.875  1.00 22.28    B   N
ATOM  2020 CA  MET B   1      4.509 104.211  56.478  1.00 22.89    B   C
ATOM  2021 N   LYS B   2      6.057 102.479  57.148  1.00 22.63    B   N
ATOM  2022 CA  LYS B   2      7.185 101.568  57.010  1.00 21.27    B   C
ATOM  2023 CB  LYS B   2      8.060 101.591  58.260  1.00 21.29    B   C
ATOM  2024 CG  LYS B   2      9.273 100.675  58.156  1.00 18.62    B   C
ATOM  2025 CD  LYS B   2     10.097 100.705  59.419  1.00 18.80    B   C
ATOM  2026 CE  LYS B   2     11.414  99.983  59.213  1.00 19.94    B   C
ATOM  2027 NZ  LYS B   2     12.203  99.908  60.474  1.00 21.20    B   N
ATOM  2028 C   LYS B   2      6.610 100.169  56.822  1.00 19.67    B   C
ATOM  2029 O   LYS B   2      5.903  99.661  57.692  1.00 20.03    B   O
ATOM  2030 N   ILE B   3      6.915  99.545  55.689  1.00 18.60    B   N
ATOM  2031 CA  ILE B   3      6.395  98.213  55.410  1.00 16.13    B   C
ATOM  2032 CB  ILE B   3      5.409  98.250  54.232  1.00 18.20    B   C
ATOM  2033 CG2 ILE B   3      4.281  99.237  54.516  1.00 15.72    B   C
ATOM  2034 CG1 ILE B   3      6.156  98.669  52.964  1.00 17.99    B   C
ATOM  2035 CD1 ILE B   3      5.909  97.772  51.772  1.00 20.13    B   C
ATOM  2036 C   ILE B   3      7.476  97.190  55.062  1.00 17.01    B   C
ATOM  2037 O   ILE B   3      8.637  97.535  54.820  1.00 13.35    B   O
ATOM  2038 N   GLY B   4      7.072  95.924  55.046  1.00 15.79    B   N
ATOM  2039 CA  GLY B   4      7.982  94.859  54.678  1.00 13.12    B   C
ATOM  2040 C   GLY B   4      7.474  94.217  53.401  1.00 12.84    B   C
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Figure 4KK

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ATOM  2041  O   GLY B  4      6.271  94.248  53.123  1.00 12.27      B   O
ATOM  2042  N   VAL B  5      8.387  93.670  52.602  1.00 11.41      B   N
ATOM  2043  CA  VAL B  5      8.024  92.982  51.362  1.00 12.46      B   C
ATOM  2044  CB  VAL B  5      8.471  93.755  50.092  1.00 11.43      B   C
ATOM  2045  CG1 VAL B  5      8.281  92.886  48.860  1.00 10.57      B   C
ATOM  2046  CG2 VAL B  5      7.646  95.026  49.938  1.00 13.41      B   C
ATOM  2047  C   VAL B  5      8.745  91.641  51.404  1.00 11.84      B   C
ATOM  2048  O   VAL B  5      9.964  91.591  51.565  1.00 13.84      B   O
ATOM  2049  N   PHE B  6      7.989  90.559  51.277  1.00 11.52      B   N
ATOM  2050  CA  PHE B  6      8.571  89.222  51.330  1.00 12.00      B   C
ATOM  2051  CB  PHE B  6      7.930  88.429  52.471  1.00 14.01      B   C
ATOM  2052  CG  PHE B  6      8.313  86.975  52.485  1.00 15.68      B   C
ATOM  2053  CD1 PHE B  6      9.650  86.598  52.576  1.00 15.79      B   C
ATOM  2054  CD2 PHE B  6      7.340  85.983  52.403  1.00 17.28      B   C
ATOM  2055  CE1 PHE B  6     10.017  85.251  52.584  1.00 15.22      B   C
ATOM  2056  CE2 PHE B  6      7.699  84.628  52.411  1.00 18.59      B   C
ATOM  2057  CZ  PHE B  6      9.044  84.268  52.502  1.00 15.23      B   C
ATOM  2058  C   PHE B  6      8.440  88.410  50.046  1.00 12.99      B   C
ATOM  2059  O   PHE B  6      7.396  88.412  49.400  1.00 13.52      B   O
ATOM  2060  N   ASP B  7      9.512  87.707  49.695  1.00 13.22      B   N
ATOM  2061  CA  ASP B  7      9.533  86.839  48.523  1.00 12.28      B   C
ATOM  2062  CB  ASP B  7      9.914  87.600  47.254  1.00 12.10      B   C
ATOM  2063  CG  ASP B  7      9.838  86.727  46.018  1.00 11.16      B   C
ATOM  2064  OD1 ASP B  7      8.773  86.111  45.800  1.00 11.05      B   O
ATOM  2065  OD2 ASP B  7     10.835  86.652  45.265  1.00 15.46      B   O
ATOM  2066  C   ASP B  7     10.544  85.730  48.749  1.00 12.97      B   C
ATOM  2067  O   ASP B  7     11.402  85.831  49.626  1.00 14.91      B   O
ATOM  2068  N   SER B  8     10.444  84.670  47.953  1.00 13.64      B   N
ATOM  2069  CA  SER B  8     11.367  83.551  48.076  1.00 13.32      B   C
ATOM  2070  CB  SER B  8     10.870  82.357  47.246  1.00 11.76      B   C
ATOM  2071  OG  SER B  8     10.643  82.716  45.892  1.00 12.59      B   O
ATOM  2072  C   SER B  8     12.760  83.979  47.618  1.00 12.86      B   C
ATOM  2073  O   SER B  8     13.760  83.328  47.931  1.00 15.56      B   O
ATOM  2074  N   GLY B  9     12.826  85.088  46.888  1.00 14.15      B   N
ATOM  2075  CA  GLY B  9     14.113  85.565  46.418  1.00 11.94      B   C
ATOM  2076  C   GLY B  9     14.060  86.923  45.751  1.00 13.28      B   C
ATOM  2077  O   GLY B  9     13.420  87.855  46.255  1.00 11.42      B   O
ATOM  2078  N   VAL B 10     14.731  87.031  44.608  1.00 11.70      B   N
ATOM  2079  CA  VAL B 10     14.793  88.283  43.848  1.00 13.19      B   C
ATOM  2080  CB  VAL B 10     16.035  88.301  42.931  1.00 11.94      B   C
ATOM  2081  CG1 VAL B 10     15.956  87.149  41.948  1.00 17.01      B   C
ATOM  2082  CG2 VAL B 10     16.148  89.633  42.200  1.00 12.63      B   C
ATOM  2083  C   VAL B 10     13.546  88.495  42.995  1.00 12.34      B   C
ATOM  2084  O   VAL B 10     13.267  89.604  42.550  1.00 14.01      B   O
ATOM  2085  N   GLY B 11     12.794  87.426  42.768  1.00 12.08      B   N
ATOM  2086  CA  GLY B 11     11.591  87.540  41.957  1.00 14.90      B   C
ATOM  2087  C   GLY B 11     10.634  88.640  42.373  1.00 12.77      B   C
ATOM  2088  O   GLY B 11     10.004  89.278  41.524  1.00 13.23      B   O
ATOM  2089  N   GLY B 12     10.524  88.861  43.679  1.00 13.56      B   N
ATOM  2090  CA  GLY B 12      9.639  89.887  44.198  1.00 15.76      B   C
ATOM  2091  C   GLY B 12      9.917  91.279  43.659  1.00 15.26      B   C
ATOM  2092  O   GLY B 12      9.141  92.213  43.899  1.00 15.12      B   O
ATOM  2093  N   PHE B 13     11.024  91.426  42.937  1.00 12.59      B   N
ATOM  2094  CA  PHE B 13     11.376  92.713  42.360  1.00 14.03      B   C
ATOM  2095  CB  PHE B 13     12.702  92.620  41.589  1.00 14.04      B   C
ATOM  2096  CG  PHE B 13     13.929  92.823  42.446  1.00 14.87      B   C
ATOM  2097  CD1 PHE B 13     15.133  93.231  41.868  1.00 16.32      B   C
ATOM  2098  CD2 PHE B 13     13.883  92.629  43.823  1.00 14.64      B   C
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Figure 4LL

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ATOM  2099 CE1 PHE B 13     16.272  93.448  42.651  1.00 13.70    B   C
ATOM  2100 CE2 PHE B 13     15.013  92.842  44.614  1.00 13.54    B   C
ATOM  2101 CZ  PHE B 13     16.210  93.254  44.025  1.00 15.35    B   C
ATOM  2102 C   PHE B 13     10.260  93.184  41.425  1.00 14.72    B   C
ATOM  2103 O   PHE B 13     10.013  94.380  41.301  1.00 12.42    B   O
ATOM  2104 N   SER B 14      9.580  92.243  40.775  1.00 14.71    B   N
ATOM  2105 CA  SER B 14      8.494  92.600  39.860  1.00 14.65    B   C
ATOM  2106 CB  SER B 14      7.918  91.349  39.187  1.00 14.09    B   C
ATOM  2107 OG  SER B 14      7.405  90.436  40.135  1.00 13.06    B   O
ATOM  2108 C   SER B 14      7.380  93.355  40.587  1.00 14.07    B   C
ATOM  2109 O   SER B 14      6.688  94.187  39.994  1.00 13.89    B   O
ATOM  2110 N   VAL B 15      7.212  93.064  41.872  1.00 14.55    B   N
ATOM  2111 CA  VAL B 15      6.196  93.737  42.675  1.00 14.09    B   C
ATOM  2112 CB  VAL B 15      5.675  92.827  43.814  1.00 12.74    B   C
ATOM  2113 CG1 VAL B 15      4.705  93.600  44.698  1.00 13.09    B   C
ATOM  2114 CG2 VAL B 15      4.971  91.604  43.224  1.00 11.77    B   C
ATOM  2115 C   VAL B 15      6.789  95.003  43.283  1.00 14.70    B   C
ATOM  2116 O   VAL B 15      6.145  96.052  43.307  1.00 13.74    B   O
ATOM  2117 N   LEU B 16      8.022  94.903  43.769  1.00 13.69    B   N
ATOM  2118 CA  LEU B 16      8.679  96.048  44.384  1.00 14.26    B   C
ATOM  2119 CB  LEU B 16     10.082  95.662  44.863  1.00 13.66    B   C
ATOM  2120 CG  LEU B 16     10.940  96.793  45.448  1.00 14.21    B   C
ATOM  2121 CD1 LEU B 16     10.201  97.451  46.605  1.00 12.59    B   C
ATOM  2122 CD2 LEU B 16     12.280  96.242  45.905  1.00 12.19    B   C
ATOM  2123 C   LEU B 16      8.757  97.212  43.401  1.00 16.29    B   C
ATOM  2124 O   LEU B 16      8.614  98.373  43.787  1.00 16.57    B   O
ATOM  2125 N   LYS B 17      8.984  96.896  42.129  1.00 17.51    B   N
ATOM  2126 CA  LYS B 17      9.069  97.927  41.099  1.00 19.45    B   C
ATOM  2127 CB  LYS B 17      9.349  97.298  39.733  1.00 19.95    B   C
ATOM  2128 CG  LYS B 17      9.302  98.291  38.578  1.00 24.40    B   C
ATOM  2129 CD  LYS B 17      9.568  97.608  37.245  1.00 29.79    B   C
ATOM  2130 CE  LYS B 17      9.472  98.586  36.081  1.00 33.15    B   C
ATOM  2131 NZ  LYS B 17      9.808  97.925  34.784  1.00 35.04    B   N
ATOM  2132 C   LYS B 17      7.769  98.722  41.038  1.00 19.40    B   C
ATOM  2133 O   LYS B 17      7.788  99.950  40.985  1.00 18.81    B   O
ATOM  2134 N   SER B 18      6.642  98.018  41.042  1.00 18.29    B   N
ATOM  2135 CA  SER B 18      5.344  98.675  40.997  1.00 18.21    B   C
ATOM  2136 CB  SER B 18      4.221  97.636  40.941  1.00 17.21    B   C
ATOM  2137 OG  SER B 18      4.357  96.808  39.798  1.00 17.80    B   O
ATOM  2138 C   SER B 18      5.162  99.561  42.222  1.00 19.88    B   C
ATOM  2139 O   SER B 18      4.720 100.703  42.112  1.00 17.77    B   O
ATOM  2140 N   LEU B 19      5.510  99.030  43.391  1.00 19.41    B   N
ATOM  2141 CA  LEU B 19      5.379  99.785  44.629  1.00 19.33    B   C
ATOM  2142 CB  LEU B 19      5.839  98.936  45.817  1.00 18.90    B   C
ATOM  2143 CG  LEU B 19      5.085  97.622  46.027  1.00 20.11    B   C
ATOM  2144 CD1 LEU B 19      5.701  96.850  47.188  1.00 18.40    B   C
ATOM  2145 CD2 LEU B 19      3.612  97.919  46.289  1.00 17.29    B   C
ATOM  2146 C   LEU B 19      6.205 101.063  44.564  1.00 18.96    B   C
ATOM  2147 O   LEU B 19      5.722 102.145  44.897  1.00 19.77    B   O
ATOM  2148 N   LEU B 20      7.455 100.930  44.136  1.00 19.62    B   N
ATOM  2149 CA  LEU B 20      8.355 102.071  44.024  1.00 20.54    B   C
ATOM  2150 CB  LEU B 20      9.736 101.605  43.548  1.00 19.03    B   C
ATOM  2151 CG  LEU B 20     10.562 100.763  44.529  1.00 21.61    B   C
ATOM  2152 CD1 LEU B 20     11.789 100.217  43.824  1.00 17.66    B   C
ATOM  2153 CD2 LEU B 20     10.968 101.613  45.731  1.00 17.70    B   C
ATOM  2154 C   LEU B 20      7.821 103.148  43.077  1.00 21.80    B   C
ATOM  2155 O   LEU B 20      7.864 104.334  43.397  1.00 24.32    B   O
ATOM  2156 N   LYS B 21      7.321 102.736  41.916  1.00 22.92    B   N
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Figure 4MM

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ATOM  2157  CA  LYS B  21      6.789 103.680  40.932  1.00 25.60      B   C
ATOM  2158  CB  LYS B  21      6.334 102.934  39.671  1.00 29.64      B   C
ATOM  2159  CG  LYS B  21      7.412 102.050  39.049  1.00 39.78      B   C
ATOM  2160  CD  LYS B  21      6.819 100.964  38.139  1.00 45.78      B   C
ATOM  2161  CE  LYS B  21      6.314 101.521  36.813  1.00 49.52      B   C
ATOM  2162  NZ  LYS B  21      7.428 101.970  35.926  1.00 52.40      B   N
ATOM  2163  C   LYS B  21     5.610 104.455  41.513  1.00 24.12      B   C
ATOM  2164  O   LYS B  21     5.461 105.652  41.270  1.00 21.99      B   O
ATOM  2165  N   ALA B  22     4.775 103.762  42.281  1.00 22.32      B   N
ATOM  2166  CA  ALA B  22      3.602 104.378  42.889  1.00 23.02      B   C
ATOM  2167  CB  ALA B  22      2.619 103.299  43.321  1.00 21.51      B   C
ATOM  2168  C   ALA B  22     3.950 105.279  44.074  1.00 25.48      B   C
ATOM  2169  O   ALA B  22     3.082 105.975  44.602  1.00 26.34      B   O
ATOM  2170  N   ARG B  23     5.214 105.264  44.489  1.00 26.06      B   N
ATOM  2171  CA  ARG B  23      5.674 106.090  45.606  1.00 28.97      B   C
ATOM  2172  CB  ARG B  23      5.794 107.556  45.170  1.00 33.33      B   C
ATOM  2173  CG  ARG B  23      6.504 107.770  43.850  1.00 41.37      B   C
ATOM  2174  CD  ARG B  23      6.349 109.205  43.378  1.00 47.44      B   C
ATOM  2175  NE  ARG B  23      6.782 109.366  41.992  1.00 56.48      B   N
ATOM  2176  CZ  ARG B  23      6.602 110.472  41.275  1.00 59.85      B   C
ATOM  2177  NH1 ARG B  23      5.998 111.520  41.819  1.00 63.01      B   N
ATOM  2178  NH2 ARG B  23      7.019 110.529  40.015  1.00 61.13      B   N
ATOM  2179  C   ARG B  23     4.697 106.012  46.774  1.00 27.89      B   C
ATOM  2180  O   ARG B  23     4.246 107.042  47.276  1.00 27.91      B   O
ATOM  2181  N   LEU B  24     4.373 104.797  47.205  1.00 25.94      B   N
ATOM  2182  CA  LEU B  24      3.430 104.611  48.303  1.00 24.48      B   C
ATOM  2183  CB  LEU B  24      2.653 103.301  48.118  1.00 22.57      B   C
ATOM  2184  CG  LEU B  24      1.822 103.103  46.847  1.00 24.84      B   C
ATOM  2185  CD1 LEU B  24      1.067 101.779  46.942  1.00 23.08      B   C
ATOM  2186  CD2 LEU B  24      0.842 104.266  46.671  1.00 23.49      B   C
ATOM  2187  C   LEU B  24     4.048 104.617  49.699  1.00 24.22      B   C
ATOM  2188  O   LEU B  24     3.445 105.126  50.641  1.00 25.35      B   O
ATOM  2189  N   PHE B  25     5.250 104.068  49.842  1.00 25.14      B   N
ATOM  2190  CA  PHE B  25      5.865 103.997  51.161  1.00 25.20      B   C
ATOM  2191  CB  PHE B  25      6.078 102.531  51.530  1.00 24.64      B   C
ATOM  2192  CG  PHE B  25      4.886 101.665  51.251  1.00 23.70      B   C
ATOM  2193  CD1 PHE B  25      4.849 100.851  50.123  1.00 23.04      B   C
ATOM  2194  CD2 PHE B  25      3.788 101.685  52.098  1.00 22.47      B   C
ATOM  2195  CE1 PHE B  25      3.729 100.070  49.845  1.00 20.01      B   C
ATOM  2196  CE2 PHE B  25      2.666 100.910  51.828  1.00 22.66      B   C
ATOM  2197  CZ  PHE B  25      2.637 100.100  50.697  1.00 21.24      B   C
ATOM  2198  C   PHE B  25     7.164 104.758  51.361  1.00 25.96      B   C
ATOM  2199  O   PHE B  25     8.020 104.796  50.482  1.00 28.54      B   O
ATOM  2200  N   ASP B  26     7.308 105.355  52.540  1.00 26.35      B   N
ATOM  2201  CA  ASP B  26      8.512 106.108  52.872  1.00 28.67      B   C
ATOM  2202  CB  ASP B  26      8.300 106.958  54.130  1.00 31.57      B   C
ATOM  2203  CG  ASP B  26      7.335 108.101  53.907  1.00 33.21      B   C
ATOM  2204  OD1 ASP B  26      7.429 108.753  52.844  1.00 33.40      B   O
ATOM  2205  OD2 ASP B  26      6.495 108.352  54.800  1.00 37.72      B   O
ATOM  2206  C   ASP B  26     9.697 105.186  53.109  1.00 25.51      B   C
ATOM  2207  O   ASP B  26     10.840 105.567  52.877  1.00 22.85      B   O
ATOM  2208  N   GLU B  27     9.421 103.974  53.581  1.00 24.08      B   N
ATOM  2209  CA  GLU B  27      10.483 103.013  53.859  1.00 21.60      B   C
ATOM  2210  CB  GLU B  27      10.964 103.179  55.305  1.00 22.98      B   C
ATOM  2211  CG  GLU B  27      11.869 102.071  55.800  1.00 25.73      B   C
ATOM  2212  CD  GLU B  27      12.636 102.459  57.051  1.00 30.40      B   C
ATOM  2213  OE1 GLU B  27      12.088 103.219  57.883  1.00 28.18      B   O
ATOM  2214  OE2 GLU B  27      13.785 101.993  57.207  1.00 28.75      B   O
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Figure 4NN

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ATOM  2215  C  GLU B 27    10.036 101.576  53.601  1.00 19.70    B   C
ATOM  2216  O  GLU B 27     8.919 101.184  53.948  1.00 17.68    B   O
ATOM  2217  N  ILE B 28    10.926 100.795  52.995  1.00 16.91    B   N
ATOM  2218  CA ILE B 28    10.630  99.407  52.651  1.00 14.07    B   C
ATOM  2219  CB ILE B 28    10.394  99.276  51.121  1.00 15.11    B   C
ATOM  2220  CG2 ILE B 28    10.279  97.816  50.711  1.00 15.06    B   C
ATOM  2221  CG1 ILE B 28     9.124 100.034  50.732  1.00 15.08    B   C
ATOM  2222  CD1 ILE B 28     8.920 100.162  49.218  1.00 17.55    B   C
ATOM  2223  C  ILE B 28    11.740  98.446  53.069  1.00 14.73    B   C
ATOM  2224  O  ILE B 28    12.925  98.694  52.825  1.00 14.43    B   O
ATOM  2225  N  ILE B 29    11.348  97.357  53.720  1.00 13.73    B   N
ATOM  2226  CA ILE B 29    12.299  96.338  54.143  1.00 15.11    B   C
ATOM  2227  CB ILE B 29    12.113  95.957  55.636  1.00 14.64    B   C
ATOM  2228  CG2 ILE B 29    13.231  95.012  56.077  1.00 13.07    B   C
ATOM  2229  CG1 ILE B 29    12.129  97.214  56.521  1.00 16.50    B   C
ATOM  2230  CD1 ILE B 29    13.462  97.949  56.554  1.00 12.57    B   C
ATOM  2231  C  ILE B 29    11.989  95.121  53.262  1.00 14.26    B   C
ATOM  2232  O  ILE B 29    10.960  94.460  53.438  1.00 16.06    B   O
ATOM  2233  N  TYR B 30    12.857  94.855  52.293  1.00 12.97    B   N
ATOM  2234  CA TYR B 30    12.667  93.728  51.382  1.00 12.66    B   C
ATOM  2235  CB TYR B 30    13.095  94.117  49.957  1.00 11.95    B   C
ATOM  2236  CG TYR B 30    12.831  93.042  48.913  1.00 11.71    B   C
ATOM  2237  CD1 TYR B 30    11.703  93.097  48.096  1.00  9.69    B   C
ATOM  2238  CE1 TYR B 30    11.441  92.100  47.149  1.00 12.54    B   C
ATOM  2239  CD2 TYR B 30    13.700  91.958  48.762  1.00 12.15    B   C
ATOM  2240  CE2 TYR B 30    13.449  90.953  47.817  1.00 14.27    B   C
ATOM  2241  CZ  TYR B 30    12.319  91.033  47.014  1.00 14.57    B   C
ATOM  2242  OH  TYR B 30    12.078  90.061  46.070  1.00 11.66    B   O
ATOM  2243  C  TYR B 30    13.473  92.516  51.842  1.00 15.13    B   C
ATOM  2244  O  TYR B 30    14.673  92.624  52.115  1.00 17.82    B   O
ATOM  2245  N  TYR B 31    12.812  91.364  51.932  1.00 13.53    B   N
ATOM  2246  CA TYR B 31    13.488  90.144  52.350  1.00 13.30    B   C
ATOM  2247  CB TYR B 31    13.063  89.742  53.773  1.00 14.35    B   C
ATOM  2248  CG TYR B 31    13.588  88.381  54.209  1.00 13.93    B   C
ATOM  2249  CD1 TYR B 31    14.955  88.143  54.318  1.00 13.81    B   C
ATOM  2250  CE1 TYR B 31    15.446  86.887  54.682  1.00 16.52    B   C
ATOM  2251  CD2 TYR B 31    12.712  87.326  54.481  1.00 15.49    B   C
ATOM  2252  CE2 TYR B 31    13.191  86.064  54.850  1.00 17.62    B   C
ATOM  2253  CZ  TYR B 31    14.563  85.852  54.946  1.00 14.49    B   C
ATOM  2254  OH  TYR B 31    15.047  84.611  55.304  1.00 14.75    B   O
ATOM  2255  C  TYR B 31    13.188  89.005  51.382  1.00 11.69    B   C
ATOM  2256  O  TYR B 31    12.032  88.657  51.153  1.00 12.79    B   O
ATOM  2257  N  GLY B 32    14.246  88.440  50.812  1.00 12.78    B   N
ATOM  2258  CA GLY B 32    14.093  87.327  49.896  1.00 11.28    B   C
ATOM  2259  C  GLY B 32    14.761  86.117  50.522  1.00 13.78    B   C
ATOM  2260  O  GLY B 32    15.950  86.162  50.839  1.00 11.17    B   O
ATOM  2261  N  ASP B 33    14.002  85.040  50.710  1.00 14.25    B   N
ATOM  2262  CA ASP B 33    14.540  83.819  51.306  1.00 15.29    B   C
ATOM  2263  CB ASP B 33    13.391  82.987  51.885  1.00 13.57    B   C
ATOM  2264  CG ASP B 33    13.871  81.730  52.589  1.00 14.42    B   C
ATOM  2265  OD1 ASP B 33    15.034  81.702  53.046  1.00 14.38    B   O
ATOM  2266  OD2 ASP B 33    13.077  80.773  52.695  1.00 14.44    B   O
ATOM  2267  C  ASP B 33    15.288  83.049  50.226  1.00 14.09    B   C
ATOM  2268  O  ASP B 33    15.027  81.867  49.980  1.00 12.43    B   O
ATOM  2269  N  SER B 34    16.238  83.739  49.597  1.00 14.94    B   N
ATOM  2270  CA SER B 34    17.016  83.186  48.490  1.00 14.92    B   C
ATOM  2271  CB SER B 34    17.941  84.268  47.908  1.00 13.20    B   C
ATOM  2272  OG SER B 34    18.886  84.714  48.863  1.00 14.39    B   O
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Figure 4OO

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ATOM  2273  C   SER B 34     17.821  81.924  48.772  1.00 14.53      B   C
ATOM  2274  O   SER B 34     18.348  81.308  47.849  1.00 12.91      B   O
ATOM  2275  N   ALA B 35     17.930  81.535  50.034  1.00 13.97      B   N
ATOM  2276  CA  ALA B 35     18.664  80.317  50.345  1.00 15.25      B   C
ATOM  2277  CB  ALA B 35     19.050  80.297  51.820  1.00 15.69      B   C
ATOM  2278  C   ALA B 35     17.801  79.101  50.023  1.00 15.43      B   C
ATOM  2279  O   ALA B 35     18.321  78.010  49.776  1.00 13.55      B   O
ATOM  2280  N   ARG B 36     16.484  79.296  50.000  1.00 13.78      B   N
ATOM  2281  CA  ARG B 36     15.567  78.185  49.777  1.00 14.22      B   C
ATOM  2282  CB  ARG B 36     14.697  78.023  51.027  1.00 13.17      B   C
ATOM  2283  CG  ARG B 36     15.541  77.986  52.303  1.00 13.84      B   C
ATOM  2284  CD  ARG B 36     14.775  77.513  53.520  1.00 16.20      B   C
ATOM  2285  NE  ARG B 36     13.830  78.511  54.012  1.00 13.15      B   N
ATOM  2286  CZ  ARG B 36     13.310  78.500  55.235  1.00 14.54      B   C
ATOM  2287  NH1 ARG B 36     13.642  77.542  56.090  1.00 13.26      B   N
ATOM  2288  NH2 ARG B 36     12.468  79.454  55.613  1.00 15.47      B   N
ATOM  2289  C   ARG B 36     14.703  78.235  48.517  1.00 14.96      B   C
ATOM  2290  O   ARG B 36     13.971  77.288  48.220  1.00 16.93      B   O
ATOM  2291  N   VAL B 37     14.791  79.328  47.770  1.00 14.56      B   N
ATOM  2292  CA  VAL B 37     14.036  79.461  46.530  1.00 15.83      B   C
ATOM  2293  CB  VAL B 37     14.327  80.840  45.875  1.00 16.33      B   C
ATOM  2294  CG1 VAL B 37     15.775  80.909  45.422  1.00 16.98      B   C
ATOM  2295  CG2 VAL B 37     13.379  81.093  44.719  1.00 16.47      B   C
ATOM  2296  C   VAL B 37     14.452  78.312  45.587  1.00 14.68      B   C
ATOM  2297  O   VAL B 37     15.615  77.895  45.575  1.00 15.45      B   O
ATOM  2298  N   PRO B 38     13.511  77.780  44.790  1.00 14.64      B   N
ATOM  2299  CD  PRO B 38     13.845  76.783  43.755  1.00 11.60      B   C
ATOM  2300  CA  PRO B 38     12.102  78.160  44.696  1.00 14.93      B   C
ATOM  2301  CB  PRO B 38     11.743  77.754  43.271  1.00 13.51      B   C
ATOM  2302  CG  PRO B 38     12.485  76.470  43.123  1.00 15.17      B   C
ATOM  2303  C   PRO B 38     11.191  77.489  45.710  1.00 15.27      B   C
ATOM  2304  O   PRO B 38     11.510  76.437  46.274  1.00 13.54      B   O
ATOM  2305  N   TYR B 39     10.043  78.118  45.915  1.00 13.69      B   N
ATOM  2306  CA  TYR B 39      9.013  77.623  46.811  1.00 13.90      B   C
ATOM  2307  CB  TYR B 39      8.268  78.798  47.444  1.00 13.72      B   C
ATOM  2308  CG  TYR B 39      8.922  79.471  48.624  1.00 10.70      B   C
ATOM  2309  CD1 TYR B 39     10.268  79.261  48.937  1.00 10.84      B   C
ATOM  2310  CE1 TYR B 39     10.860  79.906  50.023  1.00 12.25      B   C
ATOM  2311  CD2 TYR B 39      8.186  80.344  49.426  1.00 12.79      B   C
ATOM  2312  CE2 TYR B 39      8.766  80.996  50.514  1.00 12.39      B   C
ATOM  2313  CZ  TYR B 39     10.104  80.772  50.809  1.00 13.35      B   C
ATOM  2314  OH  TYR B 39     10.674  81.405  51.893  1.00 12.01      B   O
ATOM  2315  C   TYR B 39      7.997  76.821  45.987  1.00 14.02      B   C
ATOM  2316  O   TYR B 39      7.451  75.827  46.455  1.00 15.23      B   O
ATOM  2317  N   GLY B 40      7.752  77.290  44.765  1.00 16.75      B   N
ATOM  2318  CA  GLY B 40      6.768  76.686  43.874  1.00 16.84      B   C
ATOM  2319  C   GLY B 40      6.860  75.212  43.525  1.00 16.65      B   C
ATOM  2320  O   GLY B 40      5.886  74.620  43.049  1.00 14.08      B   O
ATOM  2321  N   THR B 41      8.017  74.611  43.766  1.00 15.91      B   N
ATOM  2322  CA  THR B 41      8.225  73.204  43.440  1.00 16.59      B   C
ATOM  2323  CB  THR B 41      9.636  72.990  42.900  1.00 16.07      B   C
ATOM  2324  OG1 THR B 41     10.580  73.477  43.861  1.00 15.88      B   O
ATOM  2325  CG2 THR B 41      9.817  73.737  41.592  1.00 19.86      B   C
ATOM  2326  C   THR B 41      8.072  72.320  44.659  1.00 16.87      B   C
ATOM  2327  O   THR B 41      8.245  71.099  44.584  1.00 18.68      B   O
ATOM  2328  N   LYS B 42      7.742  72.939  45.783  1.00 16.57      B   N
ATOM  2329  CA  LYS B 42      7.647  72.178  47.002  1.00 16.66      B   C
ATOM  2330  CB  LYS B 42      8.592  72.768  48.035  1.00 15.39      B   C
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Figure 4PP

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ATOM  2331 CG  LYS B 42     10.049  72.613  47.578  1.00 16.40    B   C
ATOM  2332 CD  LYS B 42     10.942  73.766  47.995  1.00 12.99    B   C
ATOM  2333 CE  LYS B 42     12.343  73.611  47.372  1.00 12.98    B   C
ATOM  2334 NZ  LYS B 42     13.246  74.754  47.688  1.00 12.01    B   N
ATOM  2335 C   LYS B 42      6.273  71.981  47.593  1.00 19.30    B   C
ATOM  2336 O   LYS B 42      5.311  72.659  47.234  1.00 19.46    B   O
ATOM  2337 N   ASP B 43      6.206  71.042  48.526  1.00 19.11    B   N
ATOM  2338 CA  ASP B 43      4.903  70.766  49.089  1.00 20.39    B   C
ATOM  2339 CB  ASP B 43      4.970  69.389  49.727  1.00 26.23    B   C
ATOM  2340 CG  ASP B 43      3.668  68.908  50.218  1.00 34.18    B   C
ATOM  2341 OD1 ASP B 43      3.032  69.628  51.023  1.00 35.73    B   O
ATOM  2342 OD2 ASP B 43      3.286  67.802  49.834  1.00 34.67    B   O
ATOM  2343 C   ASP B 43      4.324  71.860  50.037  1.00 18.74    B   C
ATOM  2344 O   ASP B 43      5.067  72.590  50.662  1.00 17.52    B   O
ATOM  2345 N   PRO B 44      2.970  71.973  50.139  1.00 16.86    B   N
ATOM  2346 CD  PRO B 44      1.945  71.249  49.366  1.00 16.70    B   C
ATOM  2347 CA  PRO B 44      2.316  72.976  51.001  1.00 15.67    B   C
ATOM  2348 CB  PRO B 44      0.838  72.608  50.910  1.00 16.57    B   C
ATOM  2349 CG  PRO B 44      0.714  72.164  49.520  1.00 15.09    B   C
ATOM  2350 C   PRO B 44      2.785  73.063  52.460  1.00 14.32    B   C
ATOM  2351 O   PRO B 44      2.975  74.159  52.984  1.00 14.18    B   O
ATOM  2352 N   THR B 45      2.968  71.928  53.125  1.00 12.56    B   N
ATOM  2353 CA  THR B 45      3.404  71.976  54.513  1.00 15.07    B   C
ATOM  2354 CB  THR B 45      3.416  70.544  55.159  1.00 14.56    B   C
ATOM  2355 OG1 THR B 45      3.473  70.671  56.582  1.00 20.74    B   O
ATOM  2356 CG2 THR B 45      4.617  69.725  54.690  1.00 16.79    B   C
ATOM  2357 C   THR B 45      4.773  72.673  54.661  1.00 13.75    B   C
ATOM  2358 O   THR B 45      5.015  73.370  55.644  1.00 15.18    B   O
ATOM  2359 N   THR B 46      5.652  72.512  53.675  1.00 14.31    B   N
ATOM  2360 CA  THR B 46      6.978  73.138  53.708  1.00 13.76    B   C
ATOM  2361 CB  THR B 46      7.908  72.534  52.625  1.00 15.70    B   C
ATOM  2362 OG1 THR B 46      8.111  71.139  52.888  1.00 16.08    B   O
ATOM  2363 CG2 THR B 46      9.257  73.237  52.611  1.00 14.55    B   C
ATOM  2364 C   THR B 46      6.874  74.645  53.463  1.00 14.40    B   C
ATOM  2365 O   THR B 46      7.538  75.450  54.120  1.00 12.91    B   O
ATOM  2366 N   ILE B 47      6.029  75.016  52.509  1.00 12.98    B   N
ATOM  2367 CA  ILE B 47      5.843  76.414  52.159  1.00 14.06    B   C
ATOM  2368 CB  ILE B 47      4.987  76.537  50.881  1.00 12.60    B   C
ATOM  2369 CG2 ILE B 47      4.790  78.005  50.517  1.00 13.35    B   C
ATOM  2370 CG1 ILE B 47      5.684  75.804  49.727  1.00 14.48    B   C
ATOM  2371 CD1 ILE B 47      4.831  75.660  48.469  1.00 13.95    B   C
ATOM  2372 C   ILE B 47      5.193  77.190  53.305  1.00 13.29    B   C
ATOM  2373 O   ILE B 47      5.588  78.314  53.610  1.00 12.68    B   O
ATOM  2374 N   LYS B 48      4.199  76.594  53.948  1.00 13.12    B   N
ATOM  2375 CA  LYS B 48      3.541  77.279  55.047  1.00 14.82    B   C
ATOM  2376 CB  LYS B 48      2.387  76.440  55.606  1.00 15.61    B   C
ATOM  2377 CG  LYS B 48      1.239  76.283  54.621  1.00 16.82    B   C
ATOM  2378 CD  LYS B 48      0.021  75.649  55.261  1.00 17.71    B   C
ATOM  2379 CE  LYS B 48     -1.123  75.558  54.259  1.00 21.58    B   C
ATOM  2380 NZ  LYS B 48     -2.370  75.047  54.891  1.00 23.95    B   N
ATOM  2381 C   LYS B 48      4.537  77.600  56.145  1.00 15.64    B   C
ATOM  2382 O   LYS B 48      4.546  78.719  56.661  1.00 14.41    B   O
ATOM  2383 N   GLN B 49      5.383  76.630  56.493  1.00 13.94    B   N
ATOM  2384 CA  GLN B 49      6.388  76.836  57.533  1.00 14.63    B   C
ATOM  2385 CB  GLN B 49      7.127  75.520  57.822  1.00 15.57    B   C
ATOM  2386 CG  GLN B 49      8.185  75.577  58.930  1.00 19.33    B   C
ATOM  2387 CD  GLN B 49      7.656  76.099  60.258  1.00 18.82    B   C
ATOM  2388 OE1 GLN B 49      6.509  75.840  60.638  1.00 17.48    B   O
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Figure 4QQ

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ATOM  2389 NE2 GLN B 49     8.498  76.826  60.977  1.00 19.58    B   N
ATOM  2390 C   GLN B 49     7.357  77.934  57.091  1.00 15.00    B   C
ATOM  2391 O   GLN B 49     7.754  78.773  57.898  1.00 15.49    B   O
ATOM  2392 N   PHE B 50     7.732  77.936  55.812  1.00 13.73    B   N
ATOM  2393 CA  PHE B 50     8.617  78.978  55.297  1.00 12.73    B   C
ATOM  2394 CB  PHE B 50     8.813  78.845  53.784  1.00 12.69    B   C
ATOM  2395 CG  PHE B 50     9.756  77.740  53.372  1.00 14.11    B   C
ATOM  2396 CD1 PHE B 50     10.540  77.073  54.310  1.00 13.47    B   C
ATOM  2397 CD2 PHE B 50     9.884  77.396  52.028  1.00 16.97    B   C
ATOM  2398 CE1 PHE B 50     11.442  76.080  53.915  1.00 14.96    B   C
ATOM  2399 CE2 PHE B 50     10.784  76.405  51.622  1.00 16.26    B   C
ATOM  2400 CZ  PHE B 50     11.563  75.747  52.569  1.00 13.12    B   C
ATOM  2401 C   PHE B 50     7.999  80.348  55.586  1.00 12.88    B   C
ATOM  2402 O   PHE B 50     8.690  81.281  55.998  1.00 14.04    B   O
ATOM  2403 N   GLY B 51     6.692  80.460  55.353  1.00 13.99    B   N
ATOM  2404 CA  GLY B 51     5.992  81.712  55.590  1.00 13.72    B   C
ATOM  2405 C   GLY B 51     6.023  82.158  57.043  1.00 14.83    B   C
ATOM  2406 O   GLY B 51     6.243  83.334  57.331  1.00 11.98    B   O
ATOM  2407 N   LEU B 52     5.788  81.227  57.966  1.00 15.32    B   N
ATOM  2408 CA  LEU B 52     5.815  81.555  59.388  1.00 18.38    B   C
ATOM  2409 CB  LEU B 52     5.525  80.320  60.248  1.00 18.53    B   C
ATOM  2410 CG  LEU B 52     4.074  79.939  60.511  1.00 24.25    B   C
ATOM  2411 CD1 LEU B 52     3.349  79.724  59.198  1.00 27.80    B   C
ATOM  2412 CD2 LEU B 52     4.037  78.679  61.371  1.00 26.46    B   C
ATOM  2413 C   LEU B 52     7.184  82.091  59.757  1.00 18.61    B   C
ATOM  2414 O   LEU B 52     7.303  83.096  60.455  1.00 21.72    B   O
ATOM  2415 N   GLU B 53     8.219  81.404  59.289  1.00 18.50    B   N
ATOM  2416 CA  GLU B 53     9.584  81.811  59.573  1.00 17.94    B   C
ATOM  2417 CB  GLU B 53     10.551  80.751  59.038  1.00 17.42    B   C
ATOM  2418 CG  GLU B 53     10.566  79.507  59.927  1.00 15.49    B   C
ATOM  2419 CD  GLU B 53     11.305  78.332  59.323  1.00 17.96    B   C
ATOM  2420 OE1 GLU B 53     12.087  78.534  58.374  1.00 18.58    B   O
ATOM  2421 OE2 GLU B 53     11.105  77.201  59.813  1.00 19.70    B   O
ATOM  2422 C   GLU B 53     9.897  83.193  59.005  1.00 18.71    B   C
ATOM  2423 O   GLU B 53     10.680  83.945  59.579  1.00 19.86    B   O
ATOM  2424 N   ALA B 54     9.271  83.537  57.885  1.00 18.53    B   N
ATOM  2425 CA  ALA B 54     9.492  84.848  57.283  1.00 16.14    B   C
ATOM  2426 CB  ALA B 54     8.744  84.951  55.954  1.00 13.28    B   C
ATOM  2427 C   ALA B 54     9.009  85.934  58.257  1.00 18.34    B   C
ATOM  2428 O   ALA B 54     9.636  86.987  58.393  1.00 16.94    B   O
ATOM  2429 N   LEU B 55     7.898  85.669  58.941  1.00 17.14    B   N
ATOM  2430 CA  LEU B 55     7.361  86.629  59.901  1.00 18.57    B   C
ATOM  2431 CB  LEU B 55     6.118  86.060  60.594  1.00 19.89    B   C
ATOM  2432 CG  LEU B 55     4.827  85.855  59.795  1.00 20.72    B   C
ATOM  2433 CD1 LEU B 55     3.771  85.221  60.706  1.00 22.99    B   C
ATOM  2434 CD2 LEU B 55     4.321  87.192  59.251  1.00 23.42    B   C
ATOM  2435 C   LEU B 55     8.405  86.999  60.956  1.00 18.71    B   C
ATOM  2436 O   LEU B 55     8.555  88.170  61.301  1.00 17.21    B   O
ATOM  2437 N   ASP B 56     9.131  86.002  61.458  1.00 18.83    B   N
ATOM  2438 CA  ASP B 56     10.151  86.241  62.474  1.00 18.36    B   C
ATOM  2439 CB  ASP B 56     10.829  84.924  62.881  1.00 21.45    B   C
ATOM  2440 CG  ASP B 56     9.875  83.958  63.581  1.00 24.57    B   C
ATOM  2441 OD1 ASP B 56     9.003  84.419  64.344  1.00 27.38    B   O
ATOM  2442 OD2 ASP B 56     10.005  82.729  63.383  1.00 26.87    B   O
ATOM  2443 C   ASP B 56     11.211  87.240  62.014  1.00 19.11    B   C
ATOM  2444 O   ASP B 56     11.669  88.082  62.792  1.00 17.72    B   O
ATOM  2445 N   PHE B 57     11.598  87.154  60.746  1.00 17.66    B   N
ATOM  2446 CA  PHE B 57     12.607  88.063  60.216  1.00 16.52    B   C
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Figure 4RR

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ATOM  2447  CB  PHE B  57     12.867  87.794  58.732  1.00 16.73      B   C
ATOM  2448  CG  PHE B  57     13.656  88.879  58.071  1.00 17.10      B   C
ATOM  2449  CD1 PHE B  57     15.035  88.958  58.247  1.00 19.76      B   C
ATOM  2450  CD2 PHE B  57     13.010  89.889  57.366  1.00 14.93      B   C
ATOM  2451  CE1 PHE B  57     15.759  90.031  57.738  1.00 19.78      B   C
ATOM  2452  CE2 PHE B  57     13.721  90.966  56.854  1.00 19.53      B   C
ATOM  2453  CZ  PHE B  57     15.100  91.039  57.041  1.00 19.60      B   C
ATOM  2454  C   PHE B  57     12.222  89.529  60.360  1.00 16.52      B   C
ATOM  2455  O   PHE B  57     13.057  90.365  60.699  1.00 18.03      B   O
ATOM  2456  N   PHE B  58     10.962  89.842  60.082  1.00 15.91      B   N
ATOM  2457  CA  PHE B  58     10.497  91.222  60.144  1.00 18.80      B   C
ATOM  2458  CB  PHE B  58      9.233  91.385  59.295  1.00 17.22      B   C
ATOM  2459  CG  PHE B  58      9.465  91.219  57.825  1.00 18.15      B   C
ATOM  2460  CD1 PHE B  58      9.217  90.004  57.199  1.00 18.00      B   C
ATOM  2461  CD2 PHE B  58      9.927  92.283  57.061  1.00 17.52      B   C
ATOM  2462  CE1 PHE B  58      9.423  89.852  55.831  1.00 16.31      B   C
ATOM  2463  CE2 PHE B  58     10.136  92.142  55.694  1.00 16.57      B   C
ATOM  2464  CZ  PHE B  58      9.884  90.924  55.077  1.00 17.04      B   C
ATOM  2465  C   PHE B  58     10.224  91.809  61.522  1.00 18.66      B   C
ATOM  2466  O   PHE B  58     10.140  93.028  61.662  1.00 21.14      B   O
ATOM  2467  N   LYS B  59     10.080  90.958  62.531  1.00 19.45      B   N
ATOM  2468  CA  LYS B  59      9.769  91.429  63.877  1.00 21.34      B   C
ATOM  2469  CB  LYS B  59      9.816  90.258  64.858  1.00 22.87      B   C
ATOM  2470  CG  LYS B  59      8.740  89.213  64.571  1.00 27.48      B   C
ATOM  2471  CD  LYS B  59      8.762  88.088  65.585  1.00 28.84      B   C
ATOM  2472  CE  LYS B  59      7.612  87.121  65.345  1.00 32.72      B   C
ATOM  2473  NZ  LYS B  59      6.308  87.829  65.430  1.00 35.68      B   N
ATOM  2474  C   LYS B  59     10.614  92.596  64.384  1.00 20.43      B   C
ATOM  2475  O   LYS B  59     10.073  93.621  64.792  1.00 19.96      B   O
ATOM  2476  N   PRO B  60     11.948  92.468  64.356  1.00 20.32      B   N
ATOM  2477  CD  PRO B  60     12.784  91.337  63.911  1.00 19.12      B   C
ATOM  2478  CA  PRO B  60     12.776  93.579  64.837  1.00 19.99      B   C
ATOM  2479  CB  PRO B  60     14.181  92.980  64.848  1.00 21.24      B   C
ATOM  2480  CG  PRO B  60     14.131  91.991  63.719  1.00 22.69      B   C
ATOM  2481  C   PRO B  60     12.690  94.859  63.995  1.00 20.53      B   C
ATOM  2482  O   PRO B  60     13.030  95.943  64.472  1.00 18.48      B   O
ATOM  2483  N   HIS B  61     12.221  94.740  62.756  1.00 18.92      B   N
ATOM  2484  CA  HIS B  61     12.116  95.896  61.871  1.00 20.35      B   C
ATOM  2485  CB  HIS B  61     12.099  95.433  60.413  1.00 19.99      B   C
ATOM  2486  CG  HIS B  61     13.409  94.875  59.953  1.00 19.89      B   C
ATOM  2487  CD2 HIS B  61     13.820  93.599  59.768  1.00 21.62      B   C
ATOM  2488  ND1 HIS B  61     14.499  95.673  59.678  1.00 21.05      B   N
ATOM  2489  CE1 HIS B  61     15.526  94.912  59.343  1.00 22.27      B   C
ATOM  2490  NE2 HIS B  61     15.142  93.649  59.390  1.00 21.05      B   N
ATOM  2491  C   HIS B  61     10.904  96.770  62.170  1.00 21.73      B   C
ATOM  2492  O   HIS B  61     10.808  97.899  61.691  1.00 22.05      B   O
ATOM  2493  N   GLU B  62      9.985  96.242  62.969  1.00 21.87      B   N
ATOM  2494  CA  GLU B  62      8.792  96.982  63.354  1.00 23.56      B   C
ATOM  2495  CB  GLU B  62      9.181  98.106  64.318  1.00 24.92      B   C
ATOM  2496  CG  GLU B  62     10.003  97.606  65.496  1.00 30.01      B   C
ATOM  2497  CD  GLU B  62     10.361  98.699  66.481  1.00 33.69      B   C
ATOM  2498  OE1 GLU B  62     10.896  99.743  66.053  1.00 35.60      B   O
ATOM  2499  OE2 GLU B  62     10.116  98.505  67.688  1.00 36.17      B   O
ATOM  2500  C   GLU B  62      8.044  97.552  62.157  1.00 22.92      B   C
ATOM  2501  O   GLU B  62      7.701  98.739  62.126  1.00 21.97      B   O
ATOM  2502  N   ILE B  63      7.795  96.706  61.164  1.00 19.69      B   N
ATOM  2503  CA  ILE B  63      7.064  97.144  59.987  1.00 18.17      B   C
ATOM  2504  CB  ILE B  63      7.236  96.149  58.825  1.00 17.22      B   C
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Figure 4SS

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ATOM  2505 CG2 ILE B  63      8.686  96.146  58.370  1.00 15.56    B   C
ATOM  2506 CG1 ILE B  63      6.817  94.746  59.269  1.00 15.21    B   C
ATOM  2507 CD1 ILE B  63      6.745  93.736  58.131  1.00 15.19    B   C
ATOM  2508 C   ILE B  63      5.590  97.258  60.375  1.00 18.21    B   C
ATOM  2509 O   ILE B  63      5.127  96.575  61.294  1.00 17.53    B   O
ATOM  2510 N   GLU B  64      4.859  98.125  59.683  1.00 16.97    B   N
ATOM  2511 CA  GLU B  64      3.445  98.349  59.985  1.00 17.61    B   C
ATOM  2512 CB  GLU B  64      3.089  99.813  59.718  1.00 18.92    B   C
ATOM  2513 CG  GLU B  64      3.934 100.801  60.499  1.00 23.07    B   C
ATOM  2514 CD  GLU B  64      3.697 102.235  60.067  1.00 26.42    B   C
ATOM  2515 OE1 GLU B  64      2.541 102.702  60.167  1.00 28.70    B   O
ATOM  2516 OE2 GLU B  64      4.667 102.889  59.624  1.00 25.35    B   O
ATOM  2517 C   GLU B  64      2.511  97.452  59.187  1.00 16.83    B   C
ATOM  2518 O   GLU B  64      1.349  97.259  59.548  1.00 16.07    B   O
ATOM  2519 N   LEU B  65      3.035  96.896  58.104  1.00 17.77    B   N
ATOM  2520 CA  LEU B  65      2.261  96.031  57.232  1.00 16.43    B   C
ATOM  2521 CB  LEU B  65      1.398  96.895  56.302  1.00 18.09    B   C
ATOM  2522 CG  LEU B  65      0.640  96.266  55.133  1.00 21.97    B   C
ATOM  2523 CD1 LEU B  65     -0.529  97.164  54.757  1.00 21.04    B   C
ATOM  2524 CD2 LEU B  65      1.572  96.066  53.944  1.00 20.71    B   C
ATOM  2525 C   LEU B  65      3.244  95.195  56.430  1.00 14.51    B   C
ATOM  2526 O   LEU B  65      4.345  95.648  56.123  1.00 12.92    B   O
ATOM  2527 N   LEU B  66      2.853  93.971  56.102  1.00 14.75    B   N
ATOM  2528 CA  LEU B  66      3.722  93.092  55.329  1.00 14.89    B   C
ATOM  2529 CB  LEU B  66      4.020  91.810  56.110  1.00 14.10    B   C
ATOM  2530 CG  LEU B  66      4.753  90.716  55.326  1.00 16.87    B   C
ATOM  2531 CD1 LEU B  66      6.149  91.214  54.949  1.00 16.67    B   C
ATOM  2532 CD2 LEU B  66      4.844  89.433  56.169  1.00 17.63    B   C
ATOM  2533 C   LEU B  66      3.091  92.722  53.995  1.00 14.55    B   C
ATOM  2534 O   LEU B  66      1.911  92.374  53.923  1.00 16.90    B   O
ATOM  2535 N   ILE B  67      3.884  92.813  52.937  1.00 14.59    B   N
ATOM  2536 CA  ILE B  67      3.422  92.451  51.610  1.00 14.92    B   C
ATOM  2537 CB  ILE B  67      3.775  93.524  50.560  1.00 17.24    B   C
ATOM  2538 CG2 ILE B  67      3.458  93.000  49.150  1.00 14.44    B   C
ATOM  2539 CG1 ILE B  67      2.995  94.815  50.846  1.00 17.41    B   C
ATOM  2540 CD1 ILE B  67      3.287  95.933  49.859  1.00 18.39    B   C
ATOM  2541 C   ILE B  67      4.117  91.159  51.207  1.00 13.22    B   C
ATOM  2542 O   ILE B  67      5.344  91.077  51.219  1.00 13.66    B   O
ATOM  2543 N   VAL B  68      3.330  90.144  50.875  1.00 13.61    B   N
ATOM  2544 CA  VAL B  68      3.898  88.878  50.430  1.00 13.77    B   C
ATOM  2545 CB  VAL B  68      3.065  87.683  50.915  1.00 12.35    B   C
ATOM  2546 CG1 VAL B  68      3.692  86.381  50.426  1.00 10.26    B   C
ATOM  2547 CG2 VAL B  68      2.991  87.699  52.438  1.00 12.86    B   C
ATOM  2548 C   VAL B  68      3.865  88.950  48.907  1.00 12.64    B   C
ATOM  2549 O   VAL B  68      2.839  88.673  48.283  1.00 14.77    B   O
ATOM  2550 N   ALA B  69      4.988  89.349  48.319  1.00 12.26    B   N
ATOM  2551 CA  ALA B  69      5.101  89.499  46.870  1.00 10.06    B   C
ATOM  2552 CB  ALA B  69      6.412  90.194  46.529  1.00  9.84    B   C
ATOM  2553 C   ALA B  69      5.027  88.163  46.147  1.00 12.35    B   C
ATOM  2554 O   ALA B  69      4.635  88.096  44.980  1.00  9.71    B   O
ATOM  2555 N   CYS B  70      5.427  87.104  46.844  1.00 11.11    B   N
ATOM  2556 CA  CYS B  70      5.418  85.766  46.273  1.00 11.24    B   C
ATOM  2557 CB  CYS B  70      6.207  84.816  47.176  1.00 11.62    B   C
ATOM  2558 SG  CYS B  70      6.347  83.142  46.504  1.00 12.64    B   S
ATOM  2559 C   CYS B  70      4.001  85.229  46.070  1.00 11.05    B   C
ATOM  2560 O   CYS B  70      3.205  85.177  47.010  1.00 11.37    B   O
ATOM  2561 N   ASN B  71      3.688  84.823  44.840  1.00 12.49    B   N
ATOM  2562 CA  ASN B  71      2.365  84.279  44.543  1.00 11.50    B   C
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Figure 4TT

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ATOM  2563 CB  ASN B  71      2.157  84.145  43.031  1.00  9.14      B   C
ATOM  2564 CG  ASN B  71      2.258  85.471  42.306  1.00 11.76      B   C
ATOM  2565 OD1 ASN B  71      3.344  86.024  42.151  1.00 10.78      B   O
ATOM  2566 ND2 ASN B  71      1.117  85.996  41.867  1.00 11.54      B   N
ATOM  2567 C   ASN B  71      2.192  82.909  45.186  1.00 12.35      B   C
ATOM  2568 O   ASN B  71      1.078  82.526  45.575  1.00  8.22      B   O
ATOM  2569 N   THR B  72      3.292  82.164  45.270  1.00 11.41      B   N
ATOM  2570 CA  THR B  72      3.257  80.831  45.863  1.00 12.16      B   C
ATOM  2571 CB  THR B  72      4.572  80.062  45.611  1.00 13.52      B   C
ATOM  2572 OG1 THR B  72      4.704  79.791  44.212  1.00 14.69      B   O
ATOM  2573 CG2 THR B  72      4.581  78.741  46.380  1.00 11.87      B   C
ATOM  2574 C   THR B  72      3.012  80.915  47.357  1.00 12.59      B   C
ATOM  2575 O   THR B  72      2.166  80.200  47.892  1.00 14.73      B   O
ATOM  2576 N   ALA B  73      3.754  81.784  48.034  1.00 13.02      B   N
ATOM  2577 CA  ALA B  73      3.576  81.953  49.471  1.00 13.51      B   C
ATOM  2578 CB  ALA B  73      4.676  82.830  50.044  1.00 13.14      B   C
ATOM  2579 C   ALA B  73      2.206  82.571  49.739  1.00 13.74      B   C
ATOM  2580 O   ALA B  73      1.580  82.278  50.752  1.00 12.89      B   O
ATOM  2581 N   SER B  74      1.751  83.437  48.830  1.00 14.66      B   N
ATOM  2582 CA  SER B  74      0.439  84.066  48.967  1.00 14.25      B   C
ATOM  2583 CB  SER B  74      0.212  85.099  47.853  1.00 13.54      B   C
ATOM  2584 OG  SER B  74      0.996  86.268  48.040  1.00 13.45      B   O
ATOM  2585 C   SER B  74     -0.655  83.002  48.877  1.00 16.32      B   C
ATOM  2586 O   SER B  74     -1.668  83.065  49.575  1.00 14.08      B   O
ATOM  2587 N   ALA B  75     -0.443  82.028  48.002  1.00 16.22      B   N
ATOM  2588 CA  ALA B  75     -1.416  80.966  47.797  1.00 17.85      B   C
ATOM  2589 CB  ALA B  75     -1.170  80.291  46.449  1.00 18.98      B   C
ATOM  2590 C   ALA B  75     -1.438  79.911  48.890  1.00 18.56      B   C
ATOM  2591 O   ALA B  75     -2.498  79.377  49.217  1.00 19.22      B   O
ATOM  2592 N   LEU B  76     -0.274  79.608  49.455  1.00 17.86      B   N
ATOM  2593 CA  LEU B  76     -0.196  78.570  50.473  1.00 19.90      B   C
ATOM  2594 CB  LEU B  76      0.921  77.580  50.131  1.00 19.60      B   C
ATOM  2595 CG  LEU B  76      0.703  76.565  49.004  1.00 21.94      B   C
ATOM  2596 CD1 LEU B  76     -0.579  75.764  49.283  1.00 19.11      B   C
ATOM  2597 CD2 LEU B  76      0.610  77.284  47.670  1.00 23.22      B   C
ATOM  2598 C   LEU B  76     -0.021  78.978  51.925  1.00 19.97      B   C
ATOM  2599 O   LEU B  76     -0.643  78.388  52.800  1.00 19.54      B   O
ATOM  2600 N   ALA B  77      0.815  79.980  52.183  1.00 20.55      B   N
ATOM  2601 CA  ALA B  77      1.111  80.380  53.559  1.00 22.00      B   C
ATOM  2602 CB  ALA B  77      2.616  80.581  53.700  1.00 20.40      B   C
ATOM  2603 C   ALA B  77      0.392  81.590  54.149  1.00 21.97      B   C
ATOM  2604 O   ALA B  77      0.420  81.792  55.365  1.00 17.66      B   O
ATOM  2605 N   LEU B  78     -0.247  82.386  53.299  1.00 23.46      B   N
ATOM  2606 CA  LEU B  78     -0.916  83.595  53.757  1.00 24.17      B   C
ATOM  2607 CB  LEU B  78     -1.634  84.271  52.583  1.00 23.46      B   C
ATOM  2608 CG  LEU B  78     -2.166  85.692  52.799  1.00 24.62      B   C
ATOM  2609 CD1 LEU B  78     -1.042  86.612  53.256  1.00 25.18      B   C
ATOM  2610 CD2 LEU B  78     -2.770  86.204  51.499  1.00 21.11      B   C
ATOM  2611 C   LEU B  78     -1.885  83.387  54.918  1.00 23.63      B   C
ATOM  2612 O   LEU B  78     -1.820  84.098  55.918  1.00 20.90      B   O
ATOM  2613 N   GLU B  79     -2.775  82.410  54.798  1.00 24.20      B   N
ATOM  2614 CA  GLU B  79     -3.744  82.171  55.856  1.00 25.27      B   C
ATOM  2615 CB  GLU B  79     -4.643  80.987  55.496  1.00 27.94      B   C
ATOM  2616 CG  GLU B  79     -5.845  80.830  56.417  1.00 34.09      B   C
ATOM  2617 CD  GLU B  79     -6.760  79.694  55.997  1.00 36.98      B   C
ATOM  2618 OE1 GLU B  79     -7.246  79.714  54.847  1.00 38.97      B   O
ATOM  2619 OE2 GLU B  79     -6.994  78.781  56.818  1.00 40.71      B   O
ATOM  2620 C   GLU B  79     -3.066  81.921  57.199  1.00 24.66      B   C
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Figure 4UU

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ATOM  2621  O   GLU B  79    -3.434  82.519  58.208  1.00 21.76    B   O
ATOM  2622  N   GLU B  80    -2.063  81.050  57.213  1.00 25.11    B   N
ATOM  2623  CA  GLU B  80    -1.367  80.740  58.455  1.00 25.16    B   C
ATOM  2624  CB  GLU B  80    -0.425  79.549  58.249  1.00 30.59    B   C
ATOM  2625  CG  GLU B  80    -0.324  78.632  59.464  1.00 36.68    B   C
ATOM  2626  CD  GLU B  80    -1.674  78.055  59.876  1.00 39.61    B   C
ATOM  2627  OE1 GLU B  80    -2.275  77.297  59.085  1.00 42.54    B   O
ATOM  2628  OE2 GLU B  80    -2.139  78.363  60.993  1.00 41.38    B   O
ATOM  2629  C   GLU B  80    -0.587  81.942  58.987  1.00 24.73    B   C
ATOM  2630  O   GLU B  80    -0.590  82.211  60.190  1.00 24.93    B   O
ATOM  2631  N   MET B  81     0.072  82.670  58.092  1.00 22.49    B   N
ATOM  2632  CA  MET B  81     0.851  83.838  58.492  1.00 20.82    B   C
ATOM  2633  CB  MET B  81     1.559  84.437  57.275  1.00 18.38    B   C
ATOM  2634  CG  MET B  81     2.671  83.563  56.717  1.00 18.17    B   C
ATOM  2635  SD  MET B  81     3.255  84.147  55.112  1.00 17.68    B   S
ATOM  2636  CE  MET B  81     4.308  85.481  55.573  1.00 12.45    B   C
ATOM  2637  C   MET B  81    -0.015  84.907  59.155  1.00 20.81    B   C
ATOM  2638  O   MET B  81     0.382  85.508  60.154  1.00 19.23    B   O
ATOM  2639  N   GLN B  82    -1.193  85.145  58.589  1.00 20.82    B   N
ATOM  2640  CA  GLN B  82    -2.111  86.145  59.129  1.00 22.97    B   C
ATOM  2641  CB  GLN B  82    -3.286  86.367  58.168  1.00 23.14    B   C
ATOM  2642  CG  GLN B  82    -2.861  86.867  56.787  1.00 22.68    B   C
ATOM  2643  CD  GLN B  82    -4.024  87.016  55.821  1.00 25.48    B   C
ATOM  2644  OE1 GLN B  82    -4.830  86.097  55.650  1.00 24.87    B   O
ATOM  2645  NE2 GLN B  82    -4.110  88.175  55.172  1.00 25.37    B   N
ATOM  2646  C   GLN B  82    -2.627  85.695  60.482  1.00 22.69    B   C
ATOM  2647  O   GLN B  82    -2.905  86.514  61.357  1.00 22.32    B   O
ATOM  2648  N   LYS B  83    -2.752  84.387  60.656  1.00 24.09    B   N
ATOM  2649  CA  LYS B  83    -3.235  83.851  61.918  1.00 25.60    B   C
ATOM  2650  CB  LYS B  83    -3.376  82.328  61.829  1.00 27.86    B   C
ATOM  2651  CG  LYS B  83    -3.766  81.658  63.141  1.00 32.07    B   C
ATOM  2652  CD  LYS B  83    -3.799  80.148  62.990  1.00 33.64    B   C
ATOM  2653  CE  LYS B  83    -4.118  79.453  64.308  1.00 38.06    B   C
ATOM  2654  NZ  LYS B  83    -4.127  77.965  64.142  1.00 38.15    B   N
ATOM  2655  C   LYS B  83    -2.298  84.218  63.065  1.00 25.66    B   C
ATOM  2656  O   LYS B  83    -2.750  84.586  64.149  1.00 23.94    B   O
ATOM  2657  N   TYR B  84    -0.993  84.134  62.825  1.00 25.08    B   N
ATOM  2658  CA  TYR B  84    -0.022  84.442  63.870  1.00 24.54    B   C
ATOM  2659  CB  TYR B  84     1.063  83.367  63.913  1.00 27.22    B   C
ATOM  2660  CG  TYR B  84     0.542  81.986  64.219  1.00 30.76    B   C
ATOM  2661  CD1 TYR B  84     0.162  81.119  63.195  1.00 31.28    B   C
ATOM  2662  CE1 TYR B  84    -0.325  79.844  63.476  1.00 34.59    B   C
ATOM  2663  CD2 TYR B  84     0.421  81.546  65.538  1.00 32.96    B   C
ATOM  2664  CE2 TYR B  84    -0.066  80.276  65.832  1.00 35.61    B   C
ATOM  2665  CZ  TYR B  84    -0.435  79.430  64.797  1.00 36.06    B   C
ATOM  2666  OH  TYR B  84    -0.904  78.167  65.089  1.00 37.33    B   O
ATOM  2667  C   TYR B  84     0.641  85.808  63.764  1.00 23.89    B   C
ATOM  2668  O   TYR B  84     1.704  86.030  64.341  1.00 25.50    B   O
ATOM  2669  N   SER B  85     0.014  86.726  63.040  1.00 22.10    B   N
ATOM  2670  CA  SER B  85     0.563  88.067  62.874  1.00 21.74    B   C
ATOM  2671  CB  SER B  85     0.884  88.323  61.397  1.00 19.79    B   C
ATOM  2672  OG  SER B  85     1.259  89.673  61.181  1.00 25.60    B   O
ATOM  2673  C   SER B  85    -0.413  89.127  63.374  1.00 21.62    B   C
ATOM  2674  O   SER B  85    -1.621  89.009  63.177  1.00 21.34    B   O
ATOM  2675  N   LYS B  86     0.107  90.157  64.031  1.00 20.33    B   N
ATOM  2676  CA  LYS B  86    -0.750  91.221  64.519  1.00 22.30    B   C
ATOM  2677  CB  LYS B  86    -0.235  91.776  65.853  1.00 25.37    B   C
ATOM  2678  CG  LYS B  86     1.182  92.304  65.826  1.00 31.07    B   C
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Figure 4VV

ATOM 2679 CD LYS B 86 1.629 92.685 67.231 1.00 35.40 B C
ATOM 2680 CE LYS B 86 1.562 91.486 68.175 1.00 35.66 B C
ATOM 2681 NZ LYS B 86 1.952 91.849 69.565 1.00 39.76 B N
ATOM 2682 C LYS B 86 -0.860 92.333 63.482 1.00 22.13 B C
ATOM 2683 O LYS B 86 -1.871 93.028 63.433 1.00 23.41 B O
ATOM 2684 N ILE B 87 0.169 92.499 62.649 1.00 20.24 B N
ATOM 2685 CA ILE B 87 0.127 93.524 61.605 1.00 18.31 B C
ATOM 2686 CB ILE B 87 1.543 94.004 61.181 1.00 16.92 B C
ATOM 2687 CG2 ILE B 87 2.244 94.688 62.359 1.00 18.70 B C
ATOM 2688 CG1 ILE B 87 2.361 92.822 60.650 1.00 17.63 B C
ATOM 2689 CD1 ILE B 87 3.721 93.203 60.117 1.00 17.00 B C
ATOM 2690 C ILE B 87 -0.559 92.921 60.384 1.00 17.72 B C
ATOM 2691 O ILE B 87 -0.553 91.707 60.193 1.00 18.08 B O
ATOM 2692 N PRO B 88 -1.173 93.762 59.542 1.00 18.77 B N
ATOM 2693 CD PRO B 88 -1.340 95.223 59.619 1.00 17.15 B C
ATOM 2694 CA PRO B 88 -1.839 93.216 58.358 1.00 19.35 B C
ATOM 2695 CB PRO B 88 -2.575 94.428 57.789 1.00 20.10 B C
ATOM 2696 CG PRO B 88 -1.691 95.572 58.194 1.00 21.95 B C
ATOM 2697 C PRO B 88 -0.844 92.619 57.360 1.00 18.71 B C
ATOM 2698 O PRO B 88 0.247 93.148 57.163 1.00 18.85 B O
ATOM 2699 N ILE B 89 -1.222 91.498 56.759 1.00 17.91 B N
ATOM 2700 CA ILE B 89 -0.387 90.848 55.757 1.00 17.91 B C
ATOM 2701 CB ILE B 89 -0.011 89.404 56.164 1.00 18.44 B C
ATOM 2702 CG2 ILE B 89 0.952 88.807 55.133 1.00 18.14 B C
ATOM 2703 CG1 ILE B 89 0.658 89.408 57.543 1.00 21.01 B C
ATOM 2704 CD1 ILE B 89 1.125 88.043 58.007 1.00 18.58 B C
ATOM 2705 C ILE B 89 -1.202 90.823 54.466 1.00 17.23 B C
ATOM 2706 O ILE B 89 -2.323 90.305 54.425 1.00 17.75 B O
ATOM 2707 N VAL B 90 -0.642 91.403 53.414 1.00 16.10 B N
ATOM 2708 CA VAL B 90 -1.334 91.467 52.141 1.00 15.66 B C
ATOM 2709 CB VAL B 90 -1.436 92.934 51.651 1.00 17.82 B C
ATOM 2710 CG1 VAL B 90 -2.241 93.001 50.351 1.00 17.58 B C
ATOM 2711 CG2 VAL B 90 -2.074 93.805 52.739 1.00 18.13 B C
ATOM 2712 C VAL B 90 -0.612 90.640 51.088 1.00 13.43 B C
ATOM 2713 O VAL B 90 0.567 90.869 50.812 1.00 14.69 B O
ATOM 2714 N GLY B 91 -1.332 89.681 50.511 1.00 13.52 B N
ATOM 2715 CA GLY B 91 -0.773 88.827 49.474 1.00 12.39 B C
ATOM 2716 C GLY B 91 -1.085 89.387 48.093 1.00 14.87 B C
ATOM 2717 O GLY B 91 -1.754 90.414 47.982 1.00 13.52 B O
ATOM 2718 N VAL B 92 -0.618 88.715 47.041 1.00 13.75 B N
ATOM 2719 CA VAL B 92 -0.840 89.190 45.676 1.00 14.98 B C
ATOM 2720 CB VAL B 92 0.447 89.066 44.819 1.00 14.03 B C
ATOM 2721 CG1 VAL B 92 1.442 90.130 45.234 1.00 9.89 B C
ATOM 2722 CG2 VAL B 92 1.056 87.672 44.978 1.00 12.60 B C
ATOM 2723 C VAL B 92 -1.975 88.505 44.922 1.00 16.65 B C
ATOM 2724 O VAL B 92 -2.194 88.786 43.746 1.00 17.87 B O
ATOM 2725 N ILE B 93 -2.702 87.616 45.585 1.00 16.90 B N
ATOM 2726 CA ILE B 93 -3.798 86.933 44.909 1.00 17.60 B C
ATOM 2727 CB ILE B 93 -3.993 85.514 45.469 1.00 18.08 B C
ATOM 2728 CG2 ILE B 93 -5.148 84.825 44.757 1.00 15.25 B C
ATOM 2729 CG1 ILE B 93 -2.693 84.722 45.291 1.00 18.10 B C
ATOM 2730 CD1 ILE B 93 -2.803 83.256 45.609 1.00 20.71 B C
ATOM 2731 C ILE B 93 -5.125 87.693 44.971 1.00 18.37 B C
ATOM 2732 O ILE B 93 -5.720 87.983 43.930 1.00 19.27 B O
ATOM 2733 N GLU B 94 -5.590 88.021 46.176 1.00 18.78 B N
ATOM 2734 CA GLU B 94 -6.859 88.742 46.315 1.00 21.11 B C
ATOM 2735 CB GLU B 94 -7.198 88.977 47.789 1.00 23.95 B C
ATOM 2736 CG GLU B 94 -7.565 87.705 48.536 1.00 28.58 B C

Figure 4WW

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ATOM  2737 CD  GLU B  94     -8.651  86.906  47.831  1.00 33.34    B   C
ATOM  2738 OE1 GLU B  94     -9.700  87.494  47.484  1.00 32.87    B   O
ATOM  2739 OE2 GLU B  94     -8.453  85.686  47.627  1.00 36.08    B   O
ATOM  2740 C   GLU B  94     -6.873  90.073  45.568  1.00 20.94    B   C
ATOM  2741 O   GLU B  94     -7.882  90.439  44.960  1.00 21.06    B   O
ATOM  2742 N   PRO B  95     -5.760  90.823  45.615  1.00 19.29    B   N
ATOM  2743 CD  PRO B  95     -4.581  90.667  46.487  1.00 17.34    B   C
ATOM  2744 CA  PRO B  95     -5.714  92.108  44.909  1.00 19.84    B   C
ATOM  2745 CB  PRO B  95     -4.301  92.603  45.196  1.00 18.81    B   C
ATOM  2746 CG  PRO B  95     -4.058  92.087  46.580  1.00 19.00    B   C
ATOM  2747 C   PRO B  95     -5.971  91.933  43.415  1.00 18.63    B   C
ATOM  2748 O   PRO B  95     -6.588  92.786  42.771  1.00 19.30    B   O
ATOM  2749 N   SER B  96     -5.485  90.824  42.867  1.00 20.23    B   N
ATOM  2750 CA  SER B  96     -5.661  90.532  41.451  1.00 19.54    B   C
ATOM  2751 CB  SER B  96     -4.752  89.380  41.032  1.00 20.19    B   C
ATOM  2752 OG  SER B  96     -3.398  89.803  41.022  1.00 21.10    B   O
ATOM  2753 C   SER B  96     -7.107  90.194  41.137  1.00 19.82    B   C
ATOM  2754 O   SER B  96     -7.623  90.554  40.076  1.00 18.36    B   O
ATOM  2755 N   ILE B  97     -7.761  89.496  42.060  1.00 19.40    B   N
ATOM  2756 CA  ILE B  97     -9.159  89.129  41.869  1.00 21.46    B   C
ATOM  2757 CB  ILE B  97     -9.702  88.310  43.066  1.00 20.75    B   C
ATOM  2758 CG2 ILE B  97    -11.185  88.032  42.872  1.00 23.74    B   C
ATOM  2759 CG1 ILE B  97     -8.929  86.996  43.205  1.00 20.33    B   C
ATOM  2760 CD1 ILE B  97     -9.130  86.028  42.048  1.00 18.39    B   C
ATOM  2761 C   ILE B  97     -9.985  90.408  41.741  1.00 20.42    B   C
ATOM  2762 O   ILE B  97    -10.881  90.502  40.904  1.00 21.88    B   O
ATOM  2763 N   LEU B  98     -9.670  91.393  42.575  1.00 22.89    B   N
ATOM  2764 CA  LEU B  98    -10.378  92.668  42.561  1.00 22.94    B   C
ATOM  2765 CB  LEU B  98     -9.918  93.539  43.734  1.00 24.42    B   C
ATOM  2766 CG  LEU B  98    -10.197  92.998  45.143  1.00 24.87    B   C
ATOM  2767 CD1 LEU B  98     -9.532  93.893  46.172  1.00 27.53    B   C
ATOM  2768 CD2 LEU B  98    -11.701  92.922  45.389  1.00 25.92    B   C
ATOM  2769 C   LEU B  98    -10.150  93.411  41.249  1.00 23.55    B   C
ATOM  2770 O   LEU B  98    -11.067  94.032  40.708  1.00 24.17    B   O
ATOM  2771 N   ALA B  99     -8.924  93.351  40.740  1.00 23.11    B   N
ATOM  2772 CA  ALA B  99     -8.594  94.025  39.491  1.00 22.89    B   C
ATOM  2773 CB  ALA B  99     -7.110  93.904  39.208  1.00 22.27    B   C
ATOM  2774 C   ALA B  99     -9.390  93.395  38.362  1.00 21.70    B   C
ATOM  2775 O   ALA B  99     -9.921  94.090  37.497  1.00 18.65    B   O
ATOM  2776 N   ILE B 100     -9.457  92.068  38.377  1.00 19.64    B   N
ATOM  2777 CA  ILE B 100    -10.190  91.331  37.363  1.00 19.82    B   C
ATOM  2778 CB  ILE B 100    -10.044  89.803  37.568  1.00 21.33    B   C
ATOM  2779 CG2 ILE B 100    -11.118  89.054  36.784  1.00 19.75    B   C
ATOM  2780 CG1 ILE B 100     -8.644  89.357  37.134  1.00 20.47    B   C
ATOM  2781 CD1 ILE B 100     -8.425  87.859  37.227  1.00 23.03    B   C
ATOM  2782 C   ILE B 100    -11.664  91.717  37.413  1.00 20.18    B   C
ATOM  2783 O   ILE B 100    -12.310  91.842  36.378  1.00 17.92    B   O
ATOM  2784 N   LYS B 101    -12.192  91.910  38.617  1.00 21.96    B   N
ATOM  2785 CA  LYS B 101    -13.594  92.296  38.755  1.00 24.71    B   C
ATOM  2786 CB  LYS B 101    -13.980  92.434  40.229  1.00 25.47    B   C
ATOM  2787 CG  LYS B 101    -14.034  91.120  40.988  1.00 30.47    B   C
ATOM  2788 CD  LYS B 101    -14.348  91.358  42.460  1.00 36.47    B   C
ATOM  2789 CE  LYS B 101    -15.720  91.992  42.654  1.00 39.30    B   C
ATOM  2790 NZ  LYS B 101    -15.973  92.336  44.087  1.00 42.89    B   N
ATOM  2791 C   LYS B 101    -13.831  93.623  38.041  1.00 24.26    B   C
ATOM  2792 O   LYS B 101    -14.846  93.797  37.369  1.00 25.28    B   O
ATOM  2793 N   ARG B 102    -12.886  94.548  38.185  1.00 23.53    B   N
ATOM  2794 CA  ARG B 102    -12.986  95.865  37.559  1.00 24.45    B   C
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Figure 4XX

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ATOM  2795 CB  ARG B 102   -11.976 96.835 38.182 1.00 24.23   B   C
ATOM  2796 CG  ARG B 102   -12.234 97.217 39.625 1.00 25.40   B   C
ATOM  2797 CD  ARG B 102   -11.276 98.316 40.054 1.00 26.37   B   C
ATOM  2798 NE  ARG B 102    -9.888 97.863 40.086 1.00 27.81   B   N
ATOM  2799 CZ  ARG B 102    -9.328 97.229 41.114 1.00 27.91   B   C
ATOM  2800 NH1 ARG B 102   -10.035 96.972 42.206 1.00 27.77   B   N
ATOM  2801 NH2 ARG B 102    -8.058 96.857 41.051 1.00 22.49   B   N
ATOM  2802 C   ARG B 102   -12.747 95.846 36.051 1.00 23.56   B   C
ATOM  2803 O   ARG B 102   -13.394 96.576 35.306 1.00 21.65   B   O
ATOM  2804 N   GLN B 103   -11.816 95.010 35.605 1.00 22.46   B   N
ATOM  2805 CA  GLN B 103   -11.474 94.951 34.189 1.00 22.58   B   C
ATOM  2806 CB  GLN B 103    -9.972 94.728 34.036 1.00 21.32   B   C
ATOM  2807 CG  GLN B 103    -9.126 95.766 34.733 1.00 22.61   B   C
ATOM  2808 CD  GLN B 103    -7.659 95.405 34.712 1.00 22.94   B   C
ATOM  2809 OE1 GLN B 103    -7.074 95.216 33.647 1.00 24.42   B   O
ATOM  2810 NE2 GLN B 103    -7.055 95.305 35.890 1.00 22.74   B   N
ATOM  2811 C   GLN B 103   -12.206 93.918 33.349 1.00 22.98   B   C
ATOM  2812 O   GLN B 103   -12.221 94.020 32.126 1.00 23.73   B   O
ATOM  2813 N   VAL B 104   -12.807 92.925 33.989 1.00 22.89   B   N
ATOM  2814 CA  VAL B 104   -13.500 91.881 33.241 1.00 24.65   B   C
ATOM  2815 CB  VAL B 104   -12.796 90.518 33.427 1.00 25.96   B   C
ATOM  2816 CG1 VAL B 104   -13.465 89.462 32.568 1.00 25.99   B   C
ATOM  2817 CG2 VAL B 104   -11.321 90.643 33.066 1.00 24.05   B   C
ATOM  2818 C   VAL B 104   -14.957 91.752 33.663 1.00 26.14   B   C
ATOM  2819 O   VAL B 104   -15.284 90.975 34.557 1.00 23.04   B   O
ATOM  2820 N   GLU B 105   -15.821 92.515 33.000 1.00 28.13   B   N
ATOM  2821 CA  GLU B 105   -17.253 92.520 33.289 1.00 31.78   B   C
ATOM  2822 CB  GLU B 105   -17.923 93.703 32.581 1.00 37.19   B   C
ATOM  2823 CG  GLU B 105   -17.318 95.053 32.940 1.00 47.02   B   C
ATOM  2824 CD  GLU B 105   -17.983 96.226 32.231 1.00 50.74   B   C
ATOM  2825 OE1 GLU B 105   -18.016 96.247 30.979 1.00 51.99   B   O
ATOM  2826 OE2 GLU B 105   -18.469 97.136 32.933 1.00 54.70   B   O
ATOM  2827 C   GLU B 105   -17.953 91.231 32.877 1.00 29.48   B   C
ATOM  2828 O   GLU B 105   -18.915 90.807 33.518 1.00 32.30   B   O
ATOM  2829 N   ASP B 106   -17.471 90.608 31.808 1.00 27.12   B   N
ATOM  2830 CA  ASP B 106   -18.067 89.377 31.310 1.00 26.01   B   C
ATOM  2831 CB  ASP B 106   -17.666 89.167 29.850 1.00 26.98   B   C
ATOM  2832 CG  ASP B 106   -18.215 87.881 29.272 1.00 28.23   B   C
ATOM  2833 OD1 ASP B 106   -19.054 87.232 29.930 1.00 28.83   B   O
ATOM  2834 OD2 ASP B 106   -17.807 87.521 28.147 1.00 31.85   B   O
ATOM  2835 C   ASP B 106   -17.666 88.168 32.147 1.00 25.85   B   C
ATOM  2836 O   ASP B 106   -16.517 87.736 32.118 1.00 24.84   B   O
ATOM  2837 N   LYS B 107   -18.628 87.626 32.890 1.00 25.49   B   N
ATOM  2838 CA  LYS B 107   -18.396 86.472 33.754 1.00 27.31   B   C
ATOM  2839 CB  LYS B 107   -19.633 86.210 34.622 1.00 29.26   B   C
ATOM  2840 CG  LYS B 107   -19.948 87.328 35.600 1.00 32.01   B   C
ATOM  2841 CD  LYS B 107   -18.757 87.611 36.512 1.00 33.91   B   C
ATOM  2842 CE  LYS B 107   -19.056 88.718 37.516 1.00 34.29   B   C
ATOM  2843 NZ  LYS B 107   -19.369 90.016 36.853 1.00 41.19   B   N
ATOM  2844 C   LYS B 107   -18.044 85.203 32.991 1.00 26.67   B   C
ATOM  2845 O   LYS B 107   -17.508 84.254 33.565 1.00 28.78   B   O
ATOM  2846 N   ASN B 108   -18.337 85.187 31.698 1.00 26.36   B   N
ATOM  2847 CA  ASN B 108   -18.059 84.019 30.875 1.00 27.30   B   C
ATOM  2848 CB  ASN B 108   -19.176 83.833 29.848 1.00 32.21   B   C
ATOM  2849 CG  ASN B 108   -20.509 83.515 30.496 1.00 37.21   B   C
ATOM  2850 OD1 ASN B 108   -20.670 82.470 31.130 1.00 41.66   B   O
ATOM  2851 ND2 ASN B 108   -21.473 84.420 30.350 1.00 39.88   B   N
ATOM  2852 C   ASN B 108   -16.719 84.106 30.160 1.00 25.00   B   C
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Figure 4YY

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ATOM  2853  O   ASN B 108    -16.318  83.173  29.467  1.00 27.12      B   O
ATOM  2854  N   ALA B 109    -16.029  85.227  30.333  1.00 22.44      B   N
ATOM  2855  CA  ALA B 109    -14.734  85.427  29.696  1.00 22.32      B   C
ATOM  2856  CB  ALA B 109    -14.179  86.795  30.062  1.00 19.60      B   C
ATOM  2857  C   ALA B 109    -13.768  84.334  30.133  1.00 21.09      B   C
ATOM  2858  O   ALA B 109    -13.580  84.107  31.326  1.00 21.33      B   O
ATOM  2859  N   PRO B 110    -13.152  83.635  29.168  1.00 21.10      B   N
ATOM  2860  CD  PRO B 110    -13.315  83.775  27.711  1.00 21.88      B   C
ATOM  2861  CA  PRO B 110    -12.201  82.562  29.485  1.00 21.55      B   C
ATOM  2862  CB  PRO B 110    -11.843  81.988  28.111  1.00 20.46      B   C
ATOM  2863  CG  PRO B 110    -13.002  82.387  27.233  1.00 23.31      B   C
ATOM  2864  C   PRO B 110    -10.974  83.142  30.190  1.00 21.39      B   C
ATOM  2865  O   PRO B 110    -10.243  83.950  29.615  1.00 20.23      B   O
ATOM  2866  N   ILE B 111    -10.757  82.731  31.433  1.00 20.74      B   N
ATOM  2867  CA  ILE B 111     -9.621  83.220  32.208  1.00 21.29      B   C
ATOM  2868  CB  ILE B 111    -10.085  83.770  33.575  1.00 18.70      B   C
ATOM  2869  CG2 ILE B 111     -8.883  84.214  34.398  1.00 19.35      B   C
ATOM  2870  CG1 ILE B 111    -11.054  84.937  33.365  1.00 17.87      B   C
ATOM  2871  CD1 ILE B 111    -11.768  85.374  34.632  1.00 13.74      B   C
ATOM  2872  C   ILE B 111     -8.618  82.096  32.439  1.00 20.50      B   C
ATOM  2873  O   ILE B 111     -8.983  81.017  32.900  1.00 21.37      B   O
ATOM  2874  N   LEU B 112     -7.358  82.354  32.107  1.00 19.57      B   N
ATOM  2875  CA  LEU B 112     -6.302  81.367  32.285  1.00 18.55      B   C
ATOM  2876  CB  LEU B 112     -5.538  81.154  30.975  1.00 17.95      B   C
ATOM  2877  CG  LEU B 112     -4.340  80.200  31.024  1.00 18.08      B   C
ATOM  2878  CD1 LEU B 112     -4.774  78.812  31.482  1.00 19.26      B   C
ATOM  2879  CD2 LEU B 112     -3.713  80.132  29.640  1.00 16.52      B   C
ATOM  2880  C   LEU B 112     -5.329  81.799  33.370  1.00 18.08      B   C
ATOM  2881  O   LEU B 112     -4.731  82.873  33.291  1.00 19.20      B   O
ATOM  2882  N   VAL B 113     -5.171  80.951  34.380  1.00 16.92      B   N
ATOM  2883  CA  VAL B 113     -4.269  81.231  35.487  1.00 16.68      B   C
ATOM  2884  CB  VAL B 113     -4.863  80.728  36.835  1.00 17.69      B   C
ATOM  2885  CG1 VAL B 113     -3.945  81.110  37.994  1.00 17.55      B   C
ATOM  2886  CG2 VAL B 113     -6.244  81.309  37.050  1.00 17.01      B   C
ATOM  2887  C   VAL B 113     -2.943  80.516  35.243  1.00 16.02      B   C
ATOM  2888  O   VAL B 113     -2.921  79.308  34.999  1.00 14.64      B   O
ATOM  2889  N   LEU B 114     -1.845  81.267  35.291  1.00 14.63      B   N
ATOM  2890  CA  LEU B 114     -0.520  80.692  35.104  1.00 13.92      B   C
ATOM  2891  CB  LEU B 114      0.247  81.395  33.979  1.00 11.65      B   C
ATOM  2892  CG  LEU B 114     -0.330  81.466  32.566  1.00 17.67      B   C
ATOM  2893  CD1 LEU B 114      0.736  82.064  31.644  1.00 16.72      B   C
ATOM  2894  CD2 LEU B 114     -0.738  80.081  32.077  1.00 17.71      B   C
ATOM  2895  C   LEU B 114      0.256  80.881  36.399  1.00 14.25      B   C
ATOM  2896  O   LEU B 114      0.210  81.947  37.005  1.00 11.47      B   O
ATOM  2897  N   GLY B 115      0.984  79.855  36.813  1.00 14.70      B   N
ATOM  2898  CA  GLY B 115      1.757  79.971  38.037  1.00 15.73      B   C
ATOM  2899  C   GLY B 115      2.608  78.746  38.289  1.00 14.74      B   C
ATOM  2900  O   GLY B 115      2.693  77.855  37.451  1.00 13.78      B   O
ATOM  2901  N   THR B 116      3.252  78.706  39.447  1.00 16.02      B   N
ATOM  2902  CA  THR B 116      4.087  77.568  39.798  1.00 15.11      B   C
ATOM  2903  CB  THR B 116      4.916  77.860  41.045  1.00 14.07      B   C
ATOM  2904  OG1 THR B 116      4.040  78.104  42.155  1.00 12.96      B   O
ATOM  2905  CG2 THR B 116      5.800  79.074  40.814  1.00 13.81      B   C
ATOM  2906  C   THR B 116      3.182  76.375  40.083  1.00 15.15      B   C
ATOM  2907  O   THR B 116      1.974  76.528  40.260  1.00 15.43      B   O
ATOM  2908  N   LYS B 117      3.768  75.189  40.124  1.00 14.92      B   N
ATOM  2909  CA  LYS B 117      2.998  73.991  40.401  1.00 16.68      B   C
ATOM  2910  CB  LYS B 117      3.926  72.776  40.462  1.00 18.20      B   C
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Figure 4ZZ

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ATOM  2911  CG  LYS B 117      3.170  71.459  40.516  1.00 28.15      B   C
ATOM  2912  CD  LYS B 117      2.286  71.334  39.280  1.00 34.68      B   C
ATOM  2913  CE  LYS B 117      1.422  70.089  39.310  1.00 37.95      B   C
ATOM  2914  NZ  LYS B 117      0.628  69.995  38.057  1.00 40.68      B   N
ATOM  2915  C   LYS B 117      2.231  74.125  41.725  1.00 15.54      B   C
ATOM  2916  O   LYS B 117      1.055  73.772  41.811  1.00 13.25      B   O
ATOM  2917  N   ALA B 118      2.896  74.648  42.753  1.00 13.55      B   N
ATOM  2918  CA  ALA B 118      2.263  74.797  44.062  1.00 13.07      B   C
ATOM  2919  CB  ALA B 118      3.294  75.271  45.092  1.00 13.77      B   C
ATOM  2920  C   ALA B 118      1.084  75.755  44.020  1.00 13.96      B   C
ATOM  2921  O   ALA B 118      0.022  75.478  44.584  1.00 12.32      B   O
ATOM  2922  N   THR B 119      1.270  76.887  43.347  1.00 12.40      B   N
ATOM  2923  CA  THR B 119      0.204  77.874  43.248  1.00 14.50      B   C
ATOM  2924  CB  THR B 119      0.698  79.159  42.534  1.00 11.89      B   C
ATOM  2925  OG1 THR B 119      1.739  79.763  43.311  1.00 13.56      B   O
ATOM  2926  CG2 THR B 119     -0.443  80.158  42.373  1.00 12.19      B   C
ATOM  2927  C   THR B 119     -1.005  77.312  42.504  1.00 12.61      B   C
ATOM  2928  O   THR B 119     -2.140  77.473  42.942  1.00 15.20      B   O
ATOM  2929  N   ILE B 120     -0.759  76.641  41.385  1.00 13.07      B   N
ATOM  2930  CA  ILE B 120     -1.847  76.080  40.594  1.00 17.11      B   C
ATOM  2931  CB  ILE B 120     -1.333  75.521  39.242  1.00 15.75      B   C
ATOM  2932  CG2 ILE B 120     -2.499  74.993  38.418  1.00 19.67      B   C
ATOM  2933  CG1 ILE B 120     -0.600  76.620  38.461  1.00 15.38      B   C
ATOM  2934  CD1 ILE B 120     -1.456  77.829  38.120  1.00 19.05      B   C
ATOM  2935  C   ILE B 120     -2.605  74.971  41.331  1.00 17.21      B   C
ATOM  2936  O   ILE B 120     -3.832  74.938  41.309  1.00 18.55      B   O
ATOM  2937  N   GLN B 121     -1.887  74.064  41.984  1.00 17.85      B   N
ATOM  2938  CA  GLN B 121     -2.554  72.983  42.700  1.00 21.02      B   C
ATOM  2939  CB  GLN B 121     -1.539  71.946  43.177  1.00 23.26      B   C
ATOM  2940  CG  GLN B 121     -0.796  71.267  42.053  1.00 31.27      B   C
ATOM  2941  CD  GLN B 121     -0.046  70.038  42.509  1.00 34.42      B   C
ATOM  2942  OE1 GLN B 121      0.702  70.078  43.488  1.00 38.77      B   O
ATOM  2943  NE2 GLN B 121     -0.237  68.933  41.797  1.00 36.80      B   N
ATOM  2944  C   GLN B 121     -3.375  73.477  43.894  1.00 21.84      B   C
ATOM  2945  O   GLN B 121     -4.297  72.795  44.345  1.00 23.51      B   O
ATOM  2946  N   SER B 122     -3.056  74.661  44.404  1.00 20.44      B   N
ATOM  2947  CA  SER B 122     -3.791  75.193  45.549  1.00 20.89      B   C
ATOM  2948  CB  SER B 122     -3.024  76.348  46.208  1.00 20.03      B   C
ATOM  2949  OG  SER B 122     -3.115  77.537  45.438  1.00 19.77      B   O
ATOM  2950  C   SER B 122     -5.178  75.687  45.152  1.00 19.13      B   C
ATOM  2951  O   SER B 122     -6.057  75.812  46.000  1.00 18.67      B   O
ATOM  2952  N   ASN B 123     -5.362  75.960  43.864  1.00 20.34      B   N
ATOM  2953  CA  ASN B 123     -6.626  76.476  43.345  1.00 21.65      B   C
ATOM  2954  CB  ASN B 123     -7.756  75.464  43.543  1.00 24.19      B   C
ATOM  2955  CG  ASN B 123     -7.662  74.302  42.583  1.00 28.22      B   C
ATOM  2956  OD1 ASN B 123     -7.618  74.492  41.368  1.00 28.03      B   O
ATOM  2957  ND2 ASN B 123     -7.632  73.087  43.121  1.00 31.95      B   N
ATOM  2958  C   ASN B 123     -6.990  77.787  44.025  1.00 20.93      B   C
ATOM  2959  O   ASN B 123     -8.162  78.160  44.098  1.00 20.81      B   O
ATOM  2960  N   ALA B 124     -5.977  78.488  44.520  1.00 18.37      B   N
ATOM  2961  CA  ALA B 124     -6.205  79.759  45.187  1.00 19.77      B   C
ATOM  2962  CB  ALA B 124     -4.872  80.387  45.588  1.00 18.94      B   C
ATOM  2963  C   ALA B 124     -6.993  80.715  44.285  1.00 18.40      B   C
ATOM  2964  O   ALA B 124     -8.032  81.239  44.685  1.00 20.72      B   O
ATOM  2965  N   TYR B 125     -6.506  80.936  43.069  1.00 19.24      B   N
ATOM  2966  CA  TYR B 125     -7.184  81.841  42.142  1.00 19.32      B   C
ATOM  2967  CB  TYR B 125     -6.331  82.091  40.892  1.00 19.37      B   C
ATOM  2968  CG  TYR B 125     -5.129  82.989  41.102  1.00 19.31      B   C
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Figure 4AAA

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ATOM  2969 CD1 TYR B 125     -3.887  82.457  41.439  1.00 17.61      B   C
ATOM  2970 CE1 TYR B 125     -2.768  83.280  41.591  1.00 18.62      B   C
ATOM  2971 CD2 TYR B 125     -5.228  84.371  40.929  1.00 17.15      B   C
ATOM  2972 CE2 TYR B 125     -4.123  85.197  41.078  1.00 16.64      B   C
ATOM  2973 CZ  TYR B 125     -2.895  84.646  41.405  1.00 17.43      B   C
ATOM  2974 OH  TYR B 125     -1.792  85.454  41.520  1.00 17.10      B   O
ATOM  2975 C   TYR B 125     -8.553  81.340  41.696  1.00 19.25      B   C
ATOM  2976 O   TYR B 125     -9.528  82.096  41.688  1.00 18.74      B   O
ATOM  2977 N   ASP B 126     -8.617  80.071  41.310  1.00 18.47      B   N
ATOM  2978 CA  ASP B 126     -9.862  79.473  40.841  1.00 19.68      B   C
ATOM  2979 CB  ASP B 126     -9.660  77.986  40.552  1.00 19.72      B   C
ATOM  2980 CG  ASP B 126     -8.455  77.720  39.671  1.00 23.51      B   C
ATOM  2981 OD1 ASP B 126     -7.341  78.138  40.042  1.00 24.96      B   O
ATOM  2982 OD2 ASP B 126     -8.621  77.085  38.609  1.00 22.93      B   O
ATOM  2983 C   ASP B 126    -10.972  79.635  41.868  1.00 21.84      B   C
ATOM  2984 O   ASP B 126    -12.076  80.077  41.541  1.00 18.17      B   O
ATOM  2985 N   ASN B 127    -10.676  79.273  43.113  1.00 21.58      B   N
ATOM  2986 CA  ASN B 127    -11.659  79.376  44.181  1.00 22.68      B   C
ATOM  2987 CB  ASN B 127    -11.081  78.839  45.495  1.00 22.98      B   C
ATOM  2988 CG  ASN B 127    -10.656  77.385  45.393  1.00 26.68      B   C
ATOM  2989 OD1 ASN B 127    -11.290  76.591  44.701  1.00 26.92      B   O
ATOM  2990 ND2 ASN B 127     -9.582  77.029  46.092  1.00 29.75      B   N
ATOM  2991 C   ASN B 127    -12.105  80.821  44.362  1.00 22.20      B   C
ATOM  2992 O   ASN B 127    -13.300  81.104  44.443  1.00 22.96      B   O
ATOM  2993 N   ALA B 128    -11.145  81.736  44.422  1.00 21.77      B   N
ATOM  2994 CA  ALA B 128    -11.465  83.149  44.587  1.00 22.81      B   C
ATOM  2995 CB  ALA B 128    -10.184  83.970  44.693  1.00 24.04      B   C
ATOM  2996 C   ALA B 128    -12.315  83.643  43.422  1.00 24.10      B   C
ATOM  2997 O   ALA B 128    -13.302  84.354  43.624  1.00 27.04      B   O
ATOM  2998 N   LEU B 129    -11.935  83.262  42.205  1.00 24.54      B   N
ATOM  2999 CA  LEU B 129    -12.672  83.664  41.012  1.00 24.58      B   C
ATOM  3000 CB  LEU B 129    -11.926  83.225  39.753  1.00 22.03      B   C
ATOM  3001 CG  LEU B 129    -10.633  83.975  39.418  1.00 24.03      B   C
ATOM  3002 CD1 LEU B 129     -9.865  83.210  38.366  1.00 22.36      B   C
ATOM  3003 CD2 LEU B 129    -10.956  85.382  38.932  1.00 22.58      B   C
ATOM  3004 C   LEU B 129    -14.078  83.070  41.005  1.00 26.08      B   C
ATOM  3005 O   LEU B 129    -15.046  83.751  40.669  1.00 26.16      B   O
ATOM  3006 N   LYS B 130    -14.185  81.795  41.365  1.00 26.80      B   N
ATOM  3007 CA  LYS B 130    -15.482  81.130  41.404  1.00 29.37      B   C
ATOM  3008 CB  LYS B 130    -15.326  79.694  41.904  1.00 32.59      B   C
ATOM  3009 CG  LYS B 130    -16.638  78.939  42.019  1.00 37.42      B   C
ATOM  3010 CD  LYS B 130    -17.337  78.877  40.675  1.00 43.42      B   C
ATOM  3011 CE  LYS B 130    -18.708  78.237  40.775  1.00 45.02      B   C
ATOM  3012 NZ  LYS B 130    -19.379  78.220  39.444  1.00 49.29      B   N
ATOM  3013 C   LYS B 130    -16.400  81.897  42.347  1.00 29.56      B   C
ATOM  3014 O   LYS B 130    -17.538  82.218  42.010  1.00 28.29      B   O
ATOM  3015 N   GLN B 131    -15.876  82.185  43.532  1.00 29.31      B   N
ATOM  3016 CA  GLN B 131    -16.599  82.911  44.559  1.00 31.88      B   C
ATOM  3017 CB  GLN B 131    -15.667  83.162  45.747  1.00 35.97      B   C
ATOM  3018 CG  GLN B 131    -16.286  83.913  46.918  1.00 45.23      B   C
ATOM  3019 CD  GLN B 131    -17.385  83.128  47.610  1.00 50.61      B   C
ATOM  3020 OE1 GLN B 131    -17.211  81.951  47.942  1.00 53.57      B   O
ATOM  3021 NE2 GLN B 131    -18.524  83.781  47.843  1.00 52.00      B   N
ATOM  3022 C   GLN B 131    -17.137  84.239  44.035  1.00 31.40      B   C
ATOM  3023 O   GLN B 131    -18.222  84.675  44.427  1.00 29.81      B   O
ATOM  3024 N   GLN B 132    -16.382  84.878  43.145  1.00 29.49      B   N
ATOM  3025 CA  GLN B 132    -16.788  86.166  42.597  1.00 29.13      B   C
ATOM  3026 CB  GLN B 132    -15.558  87.020  42.290  1.00 30.78      B   C
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Figure 4BBB

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ATOM  3027  CG  GLN B 132    -14.776  87.410  43.535  1.00 32.44    B   C
ATOM  3028  CD  GLN B 132    -15.644  88.114  44.565  1.00 35.76    B   C
ATOM  3029  OE1 GLN B 132    -16.234  89.158  44.286  1.00 35.79    B   O
ATOM  3030  NE2 GLN B 132    -15.725  87.542  45.763  1.00 34.46    B   N
ATOM  3031  C   GLN B 132    -17.682  86.079  41.368  1.00 29.17    B   C
ATOM  3032  O   GLN B 132    -17.994  87.096  40.747  1.00 28.85    B   O
ATOM  3033  N   GLY B 133    -18.075  84.864  41.004  1.00 28.71    B   N
ATOM  3034  CA  GLY B 133    -18.974  84.700  39.879  1.00 28.15    B   C
ATOM  3035  C   GLY B 133    -18.442  84.343  38.509  1.00 27.61    B   C
ATOM  3036  O   GLY B 133    -19.224  84.310  37.561  1.00 26.00    B   O
ATOM  3037  N   TYR B 134    -17.146  84.078  38.371  1.00 26.83    B   N
ATOM  3038  CA  TYR B 134    -16.627  83.721  37.056  1.00 26.16    B   C
ATOM  3039  CB  TYR B 134    -15.135  84.049  36.961  1.00 24.55    B   C
ATOM  3040  CG  TYR B 134    -14.921  85.545  36.938  1.00 22.77    B   C
ATOM  3041  CD1 TYR B 134    -14.840  86.277  38.123  1.00 22.62    B   C
ATOM  3042  CE1 TYR B 134    -14.760  87.670  38.109  1.00 23.49    B   C
ATOM  3043  CD2 TYR B 134    -14.911  86.246  35.730  1.00 24.51    B   C
ATOM  3044  CE2 TYR B 134    -14.834  87.641  35.702  1.00 25.08    B   C
ATOM  3045  CZ  TYR B 134    -14.759  88.346  36.896  1.00 23.66    B   C
ATOM  3046  OH  TYR B 134    -14.689  89.721  36.886  1.00 24.39    B   O
ATOM  3047  C   TYR B 134    -16.927  82.264  36.729  1.00 26.95    B   C
ATOM  3048  O   TYR B 134    -16.774  81.379  37.571  1.00 26.50    B   O
ATOM  3049  N   LEU B 135    -17.362  82.031  35.494  1.00 25.91    B   N
ATOM  3050  CA  LEU B 135    -17.777  80.704  35.049  1.00 28.31    B   C
ATOM  3051  CB  LEU B 135    -19.155  80.822  34.388  1.00 28.49    B   C
ATOM  3052  CG  LEU B 135    -20.131  81.733  35.139  1.00 28.21    B   C
ATOM  3053  CD1 LEU B 135    -21.343  82.031  34.272  1.00 28.13    B   C
ATOM  3054  CD2 LEU B 135    -20.527  81.077  36.455  1.00 29.07    B   C
ATOM  3055  C   LEU B 135    -16.847  79.940  34.113  1.00 27.36    B   C
ATOM  3056  O   LEU B 135    -17.066  78.758  33.855  1.00 27.87    B   O
ATOM  3057  N   ASN B 136    -15.819  80.602  33.596  1.00 28.12    B   N
ATOM  3058  CA  ASN B 136    -14.892  79.944  32.681  1.00 25.99    B   C
ATOM  3059  CB  ASN B 136    -15.053  80.520  31.276  1.00 27.18    B   C
ATOM  3060  CG  ASN B 136    -14.416  79.652  30.214  1.00 27.92    B   C
ATOM  3061  OD1 ASN B 136    -13.572  78.807  30.509  1.00 28.48    B   O
ATOM  3062  ND2 ASN B 136    -14.809  79.866  28.962  1.00 30.11    B   N
ATOM  3063  C   ASN B 136    -13.460  80.159  33.172  1.00 26.03    B   C
ATOM  3064  O   ASN B 136    -12.749  81.040  32.688  1.00 24.61    B   O
ATOM  3065  N   ILE B 137    -13.046  79.342  34.133  1.00 24.40    B   N
ATOM  3066  CA  ILE B 137    -11.715  79.451  34.716  1.00 24.19    B   C
ATOM  3067  CB  ILE B 137    -11.816  79.575  36.254  1.00 25.00    B   C
ATOM  3068  CG2 ILE B 137    -10.430  79.802  36.857  1.00 26.36    B   C
ATOM  3069  CG1 ILE B 137    -12.752  80.735  36.616  1.00 25.12    B   C
ATOM  3070  CD1 ILE B 137    -13.231  80.738  38.056  1.00 25.56    B   C
ATOM  3071  C   ILE B 137    -10.809  78.268  34.378  1.00 24.30    B   C
ATOM  3072  O   ILE B 137    -11.180  77.114  34.574  1.00 24.24    B   O
ATOM  3073  N   SER B 138    -9.620  78.570  33.865  1.00 22.99    B   N
ATOM  3074  CA  SER B 138    -8.640  77.545  33.520  1.00 23.07    B   C
ATOM  3075  CB  SER B 138    -8.357  77.547  32.016  1.00 21.90    B   C
ATOM  3076  OG  SER B 138    -9.532  77.297  31.271  1.00 28.80    B   O
ATOM  3077  C   SER B 138    -7.345  77.845  34.267  1.00 21.12    B   C
ATOM  3078  O   SER B 138    -7.104  78.986  34.675  1.00 18.88    B   O
ATOM  3079  N   HIS B 139    -6.521  76.820  34.463  1.00 20.44    B   N
ATOM  3080  CA  HIS B 139    -5.242  77.010  35.134  1.00 20.66    B   C
ATOM  3081  CB  HIS B 139    -5.343  76.712  36.639  1.00 20.23    B   C
ATOM  3082  CG  HIS B 139    -5.802  75.322  36.964  1.00 21.50    B   C
ATOM  3083  CD2 HIS B 139    -5.241  74.114  36.716  1.00 22.63    B   C
ATOM  3084  ND1 HIS B 139    -6.984  75.067  37.626  1.00 20.86    B   N
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Figure 4CCC

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ATOM  3085 CE1 HIS B 139    -7.132  73.761  37.770  1.00 23.65    B   C
ATOM  3086 NE2 HIS B 139    -6.089  73.161  37.226  1.00 23.23    B   N
ATOM  3087 C   HIS B 139    -4.172  76.148  34.488  1.00 21.34    B   C
ATOM  3088 O   HIS B 139    -4.468  75.120  33.874  1.00 21.81    B   O
ATOM  3089 N   LEU B 140    -2.922  76.578  34.614  1.00 21.36    B   N
ATOM  3090 CA  LEU B 140    -1.815  75.846  34.023  1.00 20.20    B   C
ATOM  3091 CB  LEU B 140    -1.644  76.244  32.558  1.00 21.19    B   C
ATOM  3092 CG  LEU B 140    -0.502  75.564  31.800  1.00 21.50    B   C
ATOM  3093 CD1 LEU B 140    -0.790  74.074  31.688  1.00 21.95    B   C
ATOM  3094 CD2 LEU B 140    -0.357  76.190  30.410  1.00 21.96    B   C
ATOM  3095 C   LEU B 140    -0.511  76.104  34.758  1.00 19.11    B   C
ATOM  3096 O   LEU B 140    -0.098  77.248  34.928  1.00 16.59    B   O
ATOM  3097 N   ALA B 141     0.135  75.027  35.186  1.00 19.36    B   N
ATOM  3098 CA  ALA B 141     1.405  75.133  35.887  1.00 19.87    B   C
ATOM  3099 CB  ALA B 141     1.603  73.918  36.791  1.00 21.48    B   C
ATOM  3100 C   ALA B 141     2.531  75.215  34.856  1.00 16.62    B   C
ATOM  3101 O   ALA B 141     2.912  74.214  34.261  1.00 20.61    B   O
ATOM  3102 N   THR B 142     3.049  76.415  34.630  1.00 15.84    B   N
ATOM  3103 CA  THR B 142     4.132  76.600  33.676  1.00 14.20    B   C
ATOM  3104 CB  THR B 142     3.948  77.913  32.889  1.00 13.97    B   C
ATOM  3105 OG1 THR B 142     3.814  79.003  33.806  1.00 14.25    B   O
ATOM  3106 CG2 THR B 142     2.691  77.840  32.023  1.00 13.62    B   C
ATOM  3107 C   THR B 142     5.410  76.652  34.505  1.00 14.37    B   C
ATOM  3108 O   THR B 142     6.114  77.653  34.529  1.00 13.97    B   O
ATOM  3109 N   SER B 143     5.698  75.544  35.176  1.00 15.59    B   N
ATOM  3110 CA  SER B 143     6.844  75.444  36.067  1.00 16.89    B   C
ATOM  3111 CB  SER B 143     6.971  74.013  36.591  1.00 19.31    B   C
ATOM  3112 OG  SER B 143     8.003  73.931  37.564  1.00 27.09    B   O
ATOM  3113 C   SER B 143     8.193  75.902  35.537  1.00 16.21    B   C
ATOM  3114 O   SER B 143     8.892  76.666  36.205  1.00 16.07    B   O
ATOM  3115 N   LEU B 144     8.557  75.446  34.345  1.00 15.08    B   N
ATOM  3116 CA  LEU B 144     9.850  75.783  33.759  1.00 15.48    B   C
ATOM  3117 CB  LEU B 144    10.094  74.929  32.520  1.00 15.32    B   C
ATOM  3118 CG  LEU B 144    10.215  73.436  32.827  1.00 16.70    B   C
ATOM  3119 CD1 LEU B 144    10.267  72.642  31.536  1.00 19.80    B   C
ATOM  3120 CD2 LEU B 144    11.468  73.190  33.654  1.00 19.07    B   C
ATOM  3121 C   LEU B 144    10.037  77.251  33.421  1.00 14.68    B   C
ATOM  3122 O   LEU B 144    11.145  77.678  33.098  1.00 14.35    B   O
ATOM  3123 N   PHE B 145     8.962  78.028  33.484  1.00 14.12    B   N
ATOM  3124 CA  PHE B 145     9.088  79.447  33.199  1.00 15.35    B   C
ATOM  3125 CB  PHE B 145     7.719  80.148  33.232  1.00 13.56    B   C
ATOM  3126 CG  PHE B 145     6.911  79.992  31.964  1.00 14.58    B   C
ATOM  3127 CD1 PHE B 145     5.657  80.594  31.852  1.00 13.83    B   C
ATOM  3128 CD2 PHE B 145     7.393  79.252  30.888  1.00 16.08    B   C
ATOM  3129 CE1 PHE B 145     4.899  80.461  30.688  1.00 14.15    B   C
ATOM  3130 CE2 PHE B 145     6.646  79.111  29.720  1.00 15.95    B   C
ATOM  3131 CZ  PHE B 145     5.395  79.717  29.620  1.00 14.39    B   C
ATOM  3132 C   PHE B 145    10.011  80.084  34.233  1.00 14.15    B   C
ATOM  3133 O   PHE B 145    10.821  80.942  33.896  1.00 13.84    B   O
ATOM  3134 N   VAL B 146     9.901  79.648  35.488  1.00 14.43    B   N
ATOM  3135 CA  VAL B 146    10.721  80.215  36.558  1.00 15.36    B   C
ATOM  3136 CB  VAL B 146    10.353  79.617  37.949  1.00 17.29    B   C
ATOM  3137 CG1 VAL B 146    11.367  80.065  38.995  1.00 16.50    B   C
ATOM  3138 CG2 VAL B 146     8.959  80.079  38.369  1.00 14.60    B   C
ATOM  3139 C   VAL B 146    12.229  80.086  36.329  1.00 14.39    B   C
ATOM  3140 O   VAL B 146    12.935  81.092  36.326  1.00 14.20    B   O
ATOM  3141 N   PRO B 147    12.747  78.856  36.144  1.00 14.14    B   N
ATOM  3142 CD  PRO B 147    12.141  77.519  36.269  1.00 13.43    B   C
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Figure 4DDD

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ATOM  3143 CA  PRO B 147     14.195  78.754  35.921  1.00 14.59    B   C
ATOM  3144 CB  PRO B 147     14.457  77.242  35.995  1.00 13.53    B   C
ATOM  3145 CG  PRO B 147     13.151  76.642  35.573  1.00 14.07    B   C
ATOM  3146 C   PRO B 147     14.653  79.377  34.597  1.00 13.40    B   C
ATOM  3147 O   PRO B 147     15.775  79.877  34.500  1.00 13.19    B   O
ATOM  3148 N   LEU B 148     13.796  79.355  33.577  1.00 11.38    B   N
ATOM  3149 CA  LEU B 148     14.179  79.960  32.303  1.00 12.63    B   C
ATOM  3150 CB  LEU B 148     13.100  79.751  31.232  1.00 14.70    B   C
ATOM  3151 CG  LEU B 148     13.404  78.655  30.202  1.00 12.09    B   C
ATOM  3152 CD1 LEU B 148     13.446  77.315  30.903  1.00 14.46    B   C
ATOM  3153 CD2 LEU B 148     12.341  78.649  29.106  1.00 18.20    B   C
ATOM  3154 C   LEU B 148     14.395  81.448  32.508  1.00 12.91    B   C
ATOM  3155 O   LEU B 148     15.372  82.018  32.031  1.00 12.96    B   O
ATOM  3156 N   ILE B 149     13.471  82.070  33.231  1.00 13.00    B   N
ATOM  3157 CA  ILE B 149     13.545  83.500  33.499  1.00 12.87    B   C
ATOM  3158 CB  ILE B 149     12.211  83.989  34.130  1.00 13.86    B   C
ATOM  3159 CG2 ILE B 149     12.352  85.419  34.647  1.00 12.28    B   C
ATOM  3160 CG1 ILE B 149     11.099  83.891  33.071  1.00 14.05    B   C
ATOM  3161 CD1 ILE B 149      9.694  84.067  33.608  1.00 15.21    B   C
ATOM  3162 C   ILE B 149     14.742  83.842  34.386  1.00 12.66    B   C
ATOM  3163 O   ILE B 149     15.403  84.852  34.172  1.00 11.51    B   O
ATOM  3164 N   GLU B 150     15.041  82.995  35.366  1.00 12.92    B   N
ATOM  3165 CA  GLU B 150     16.180  83.266  36.235  1.00 13.66    B   C
ATOM  3166 CB  GLU B 150     16.182  82.313  37.441  1.00 18.92    B   C
ATOM  3167 CG  GLU B 150     14.884  82.371  38.242  1.00 23.46    B   C
ATOM  3168 CD  GLU B 150     15.024  81.875  39.673  1.00 28.25    B   C
ATOM  3169 OE1 GLU B 150     15.728  80.863  39.887  1.00 30.76    B   O
ATOM  3170 OE2 GLU B 150     14.414  82.491  40.581  1.00 24.21    B   O
ATOM  3171 C   GLU B 150     17.491  83.163  35.462  1.00 13.99    B   C
ATOM  3172 O   GLU B 150     18.484  83.776  35.844  1.00 14.58    B   O
ATOM  3173 N   GLU B 151     17.500  82.403  34.370  1.00 13.36    B   N
ATOM  3174 CA  GLU B 151     18.712  82.277  33.571  1.00 16.12    B   C
ATOM  3175 CB  GLU B 151     18.863  80.861  33.006  1.00 18.99    B   C
ATOM  3176 CG  GLU B 151     20.276  80.598  32.500  1.00 25.66    B   C
ATOM  3177 CD  GLU B 151     20.615  79.128  32.403  1.00 27.80    B   C
ATOM  3178 OE1 GLU B 151     20.307  78.389  33.362  1.00 33.36    B   O
ATOM  3179 OE2 GLU B 151     21.204  78.716  31.378  1.00 24.62    B   O
ATOM  3180 C   GLU B 151     18.695  83.293  32.436  1.00 15.49    B   C
ATOM  3181 O   GLU B 151     19.515  83.243  31.522  1.00 16.76    B   O
ATOM  3182 N   SER B 152     17.746  84.218  32.514  1.00 15.83    B   N
ATOM  3183 CA  SER B 152     17.591  85.277  31.523  1.00 16.90    B   C
ATOM  3184 CB  SER B 152     18.843  86.159  31.486  1.00 16.89    B   C
ATOM  3185 OG  SER B 152     18.547  87.404  30.872  1.00 19.93    B   O
ATOM  3186 C   SER B 152     17.274  84.786  30.108  1.00 15.72    B   C
ATOM  3187 O   SER B 152     17.776  85.339  29.128  1.00 16.57    B   O
ATOM  3188 N   ILE B 153     16.452  83.746  30.003  1.00 16.59    B   N
ATOM  3189 CA  ILE B 153     16.048  83.223  28.701  1.00 16.23    B   C
ATOM  3190 CB  ILE B 153     15.840  81.688  28.747  1.00 17.80    B   C
ATOM  3191 CG2 ILE B 153     15.479  81.164  27.366  1.00 16.97    B   C
ATOM  3192 CG1 ILE B 153     17.118  81.008  29.247  1.00 18.17    B   C
ATOM  3193 CD1 ILE B 153     18.328  81.264  28.379  1.00 20.45    B   C
ATOM  3194 C   ILE B 153     14.716  83.924  28.465  1.00 17.00    B   C
ATOM  3195 O   ILE B 153     13.647  83.337  28.649  1.00 16.86    B   O
ATOM  3196 N   LEU B 154     14.802  85.192  28.074  1.00 16.13    B   N
ATOM  3197 CA  LEU B 154     13.629  86.036  27.861  1.00 17.93    B   C
ATOM  3198 CB  LEU B 154     13.891  87.412  28.475  1.00 15.30    B   C
ATOM  3199 CG  LEU B 154     14.390  87.335  29.923  1.00 14.99    B   C
ATOM  3200 CD1 LEU B 154     14.685  88.728  30.459  1.00 17.09    B   C
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Figure 4EEE

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ATOM  3201 CD2 LEU B 154    13.348  86.640  30.776  1.00 18.19    B   C
ATOM  3202 C   LEU B 154    13.188  86.204  26.413  1.00 19.02    B   C
ATOM  3203 O   LEU B 154    12.258  86.956  26.125  1.00 18.98    B   O
ATOM  3204 N   GLU B 155    13.857  85.506  25.506  1.00 19.46    B   N
ATOM  3205 CA  GLU B 155    13.520  85.579  24.093  1.00 20.61    B   C
ATOM  3206 CB  GLU B 155    14.055  86.877  23.481  1.00 23.20    B   C
ATOM  3207 CG  GLU B 155    15.563  86.894  23.285  1.00 31.50    B   C
ATOM  3208 CD  GLU B 155    16.077  88.235  22.778  1.00 39.23    B   C
ATOM  3209 OE1 GLU B 155    15.483  88.786  21.824  1.00 42.91    B   O
ATOM  3210 OE2 GLU B 155    17.084  88.734  23.328  1.00 43.36    B   O
ATOM  3211 C   GLU B 155    14.177  84.391  23.421  1.00 19.99    B   C
ATOM  3212 O   GLU B 155    14.864  83.610  24.077  1.00 21.64    B   O
ATOM  3213 N   GLY B 156    13.946  84.242  22.121  1.00 20.12    B   N
ATOM  3214 CA  GLY B 156    14.563  83.152  21.396  1.00 19.17    B   C
ATOM  3215 C   GLY B 156    13.844  81.820  21.366  1.00 20.79    B   C
ATOM  3216 O   GLY B 156    12.804  81.618  21.995  1.00 18.13    B   O
ATOM  3217 N   GLU B 157    14.451  80.898  20.626  1.00 22.19    B   N
ATOM  3218 CA  GLU B 157    13.946  79.548  20.415  1.00 21.56    B   C
ATOM  3219 CB  GLU B 157    14.952  78.782  19.553  1.00 25.02    B   C
ATOM  3220 CG  GLU B 157    14.524  77.377  19.184  1.00 35.87    B   C
ATOM  3221 CD  GLU B 157    15.499  76.703  18.231  1.00 41.09    B   C
ATOM  3222 OE1 GLU B 157    16.701  76.596  18.573  1.00 42.82    B   O
ATOM  3223 OE2 GLU B 157    15.058  76.275  17.141  1.00 42.70    B   O
ATOM  3224 C   GLU B 157    13.613  78.732  21.666  1.00 20.08    B   C
ATOM  3225 O   GLU B 157    12.588  78.044  21.702  1.00 18.27    B   O
ATOM  3226 N   LEU B 158    14.471  78.796  22.683  1.00 17.09    B   N
ATOM  3227 CA  LEU B 158    14.238  78.033  23.904  1.00 15.87    B   C
ATOM  3228 CB  LEU B 158    15.447  78.132  24.842  1.00 18.05    B   C
ATOM  3229 CG  LEU B 158    15.334  77.315  26.136  1.00 17.16    B   C
ATOM  3230 CD1 LEU B 158    14.977  75.872  25.807  1.00 15.66    B   C
ATOM  3231 CD2 LEU B 158    16.651  77.382  26.905  1.00 17.03    B   C
ATOM  3232 C   LEU B 158    12.973  78.488  24.630  1.00 16.52    B   C
ATOM  3233 O   LEU B 158    12.189  77.662  25.108  1.00 14.49    B   O
ATOM  3234 N   LEU B 159    12.775  79.799  24.727  1.00 14.92    B   N
ATOM  3235 CA  LEU B 159    11.580  80.306  25.383  1.00 14.51    B   C
ATOM  3236 CB  LEU B 159    11.660  81.823  25.578  1.00 15.13    B   C
ATOM  3237 CG  LEU B 159    10.374  82.456  26.133  1.00 16.38    B   C
ATOM  3238 CD1 LEU B 159     9.996  81.799  27.450  1.00 14.88    B   C
ATOM  3239 CD2 LEU B 159    10.574  83.955  26.326  1.00 15.09    B   C
ATOM  3240 C   LEU B 159    10.367  79.951  24.519  1.00 14.59    B   C
ATOM  3241 O   LEU B 159     9.350  79.492  25.028  1.00 13.56    B   O
ATOM  3242 N   GLU B 160    10.483  80.150  23.209  1.00 14.14    B   N
ATOM  3243 CA  GLU B 160     9.382  79.820  22.304  1.00 16.06    B   C
ATOM  3244 CB  GLU B 160     9.779  80.107  20.853  1.00 18.15    B   C
ATOM  3245 CG  GLU B 160     8.709  79.743  19.815  1.00 23.84    B   C
ATOM  3246 CD  GLU B 160     7.357  80.384  20.107  1.00 27.35    B   C
ATOM  3247 OE1 GLU B 160     7.330  81.496  20.683  1.00 24.13    B   O
ATOM  3248 OE2 GLU B 160     6.321  79.783  19.748  1.00 30.37    B   O
ATOM  3249 C   GLU B 160     8.987  78.348  22.438  1.00 15.10    B   C
ATOM  3250 O   GLU B 160     7.811  78.015  22.566  1.00 16.67    B   O
ATOM  3251 N   THR B 161     9.979  77.469  22.416  1.00 15.36    B   N
ATOM  3252 CA  THR B 161     9.720  76.037  22.518  1.00 16.10    B   C
ATOM  3253 CB  THR B 161    11.024  75.243  22.343  1.00 17.81    B   C
ATOM  3254 OG1 THR B 161    11.607  75.567  21.072  1.00 19.62    B   O
ATOM  3255 CG2 THR B 161    10.756  73.748  22.407  1.00 18.12    B   C
ATOM  3256 C   THR B 161     9.066  75.676  23.851  1.00 14.89    B   C
ATOM  3257 O   THR B 161     8.172  74.821  23.907  1.00 13.07    B   O
ATOM  3258 N   CYS B 162     9.500  76.342  24.918  1.00 12.65    B   N
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Figure 4FFF

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ATOM  3259  CA  CYS B 162      8.958  76.087  26.248  1.00 15.38      B   C
ATOM  3260  CB  CYS B 162      9.800  76.796  27.310  1.00 14.79      B   C
ATOM  3261  SG  CYS B 162      9.400  76.328  29.021  1.00 16.89      B   S
ATOM  3262  C   CYS B 162      7.505  76.557  26.341  1.00 15.60      B   C
ATOM  3263  O   CYS B 162      6.651  75.849  26.877  1.00 15.21      B   O
ATOM  3264  N   MET B 163      7.226  77.756  25.831  1.00 15.17      B   N
ATOM  3265  CA  MET B 163      5.863  78.271  25.860  1.00 15.78      B   C
ATOM  3266  CB  MET B 163      5.792  79.695  25.294  1.00 15.75      B   C
ATOM  3267  CG  MET B 163      6.424  80.767  26.162  1.00 16.77      B   C
ATOM  3268  SD  MET B 163      5.978  82.432  25.603  1.00 16.61      B   S
ATOM  3269  CE  MET B 163      6.937  82.509  24.114  1.00 14.38      B   C
ATOM  3270  C   MET B 163      4.962  77.360  25.033  1.00 14.99      B   C
ATOM  3271  O   MET B 163      3.819  77.093  25.410  1.00 15.77      B   O
ATOM  3272  N   HIS B 164      5.484  76.879  23.909  1.00 15.34      B   N
ATOM  3273  CA  HIS B 164      4.718  76.002  23.033  1.00 19.25      B   C
ATOM  3274  CB  HIS B 164      5.504  75.724  21.751  1.00 20.62      B   C
ATOM  3275  CG  HIS B 164      4.693  75.055  20.688  1.00 28.25      B   C
ATOM  3276  CD2 HIS B 164      4.779  73.817  20.146  1.00 28.01      B   C
ATOM  3277  ND1 HIS B 164      3.608  75.661  20.090  1.00 29.20      B   N
ATOM  3278  CE1 HIS B 164      3.060  74.824  19.227  1.00 29.23      B   C
ATOM  3279  NE2 HIS B 164      3.750  73.698  19.243  1.00 29.55      B   N
ATOM  3280  C   HIS B 164      4.412  74.690  23.760  1.00 19.47      B   C
ATOM  3281  O   HIS B 164      3.293  74.169  23.704  1.00 17.49      B   O
ATOM  3282  N   TYR B 165      5.419  74.169  24.449  1.00 17.68      B   N
ATOM  3283  CA  TYR B 165      5.277  72.937  25.210  1.00 16.69      B   C
ATOM  3284  CB  TYR B 165      6.578  72.655  25.969  1.00 15.68      B   C
ATOM  3285  CG  TYR B 165      6.457  71.544  26.976  1.00 17.57      B   C
ATOM  3286  CD1 TYR B 165      6.384  70.211  26.569  1.00 16.95      B   C
ATOM  3287  CE1 TYR B 165      6.216  69.191  27.498  1.00 20.45      B   C
ATOM  3288  CD2 TYR B 165      6.362  71.829  28.336  1.00 15.75      B   C
ATOM  3289  CE2 TYR B 165      6.193  70.818  29.273  1.00 17.81      B   C
ATOM  3290  CZ  TYR B 165      6.119  69.501  28.847  1.00 18.80      B   C
ATOM  3291  OH  TYR B 165      5.941  68.500  29.773  1.00 19.07      B   O
ATOM  3292  C   TYR B 165      4.101  73.027  26.193  1.00 16.83      B   C
ATOM  3293  O   TYR B 165      3.303  72.094  26.310  1.00 19.76      B   O
ATOM  3294  N   TYR B 166      3.999  74.151  26.895  1.00 16.40      B   N
ATOM  3295  CA  TYR B 166      2.931  74.369  27.864  1.00 16.70      B   C
ATOM  3296  CB  TYR B 166      3.362  75.435  28.888  1.00 13.68      B   C
ATOM  3297  CG  TYR B 166      4.354  74.961  29.930  1.00 15.63      B   C
ATOM  3298  CD1 TYR B 166      5.545  75.650  30.150  1.00 13.48      B   C
ATOM  3299  CE1 TYR B 166      6.458  75.218  31.113  1.00 17.41      B   C
ATOM  3300  CD2 TYR B 166      4.097  73.825  30.702  1.00 16.97      B   C
ATOM  3301  CE2 TYR B 166      5.001  73.387  31.668  1.00 14.41      B   C
ATOM  3302  CZ  TYR B 166      6.176  74.084  31.868  1.00 15.99      B   C
ATOM  3303  OH  TYR B 166      7.058  73.648  32.827  1.00 15.83      B   O
ATOM  3304  C   TYR B 166      1.576  74.793  27.278  1.00 17.53      B   C
ATOM  3305  O   TYR B 166      0.529  74.344  27.746  1.00 18.77      B   O
ATOM  3306  N   PHE B 167      1.599  75.651  26.260  1.00 18.80      B   N
ATOM  3307  CA  PHE B 167      0.367  76.198  25.668  1.00 19.74      B   C
ATOM  3308  CB  PHE B 167      0.660  77.589  25.115  1.00 18.42      B   C
ATOM  3309  CG  PHE B 167      1.092  78.573  26.163  1.00 17.20      B   C
ATOM  3310  CD1 PHE B 167      1.928  79.627  25.824  1.00 16.80      B   C
ATOM  3311  CD2 PHE B 167      0.635  78.472  27.482  1.00 16.87      B   C
ATOM  3312  CE1 PHE B 167      2.306  80.572  26.770  1.00 17.05      B   C
ATOM  3313  CE2 PHE B 167      1.010  79.419  28.439  1.00 17.71      B   C
ATOM  3314  CZ  PHE B 167      1.851  80.472  28.075  1.00 17.51      B   C
ATOM  3315  C   PHE B 167     -0.367  75.383  24.618  1.00 21.10      B   C
ATOM  3316  O   PHE B 167     -1.597  75.430  24.535  1.00 19.22      B   O
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Figure 4GGG

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ATOM  3317  N   THR B 168      0.403  74.657  23.812  1.00 23.27    B   N
ATOM  3318  CA  THR B 168     -0.165  73.805  22.765  1.00 26.77    B   C
ATOM  3319  CB  THR B 168      0.865  72.832  22.187  1.00 27.57    B   C
ATOM  3320  OG1 THR B 168      1.911  73.535  21.517  1.00 32.03    B   O
ATOM  3321  CG2 THR B 168      0.186  71.880  21.180  1.00 32.54    B   C
ATOM  3322  C   THR B 168     -1.363  72.944  23.205  1.00 26.77    B   C
ATOM  3323  O   THR B 168     -2.395  72.938  22.572  1.00 28.26    B   O
ATOM  3324  N   PRO B 169     -1.239  72.197  24.326  1.00 26.46    B   N
ATOM  3325  CD  PRO B 169     -0.050  72.083  25.152  1.00 26.67    B   C
ATOM  3326  CA  PRO B 169     -2.291  71.326  24.883  1.00 25.55    B   C
ATOM  3327  CB  PRO B 169     -1.610  70.668  26.066  1.00 26.50    B   C
ATOM  3328  CG  PRO B 169     -0.169  70.666  25.699  1.00 26.43    B   C
ATOM  3329  C   PRO B 169     -3.593  72.077  25.297  1.00 24.82    B   C
ATOM  3330  O   PRO B 169     -4.610  71.418  25.576  1.00 24.34    B   O
ATOM  3331  N   LEU B 170     -3.536  73.405  25.391  1.00 22.80    B   N
ATOM  3332  CA  LEU B 170     -4.729  74.167  25.761  1.00 25.50    B   C
ATOM  3333  CB  LEU B 170     -4.385  75.632  25.964  1.00 23.84    B   C
ATOM  3334  CG  LEU B 170     -3.514  75.982  27.186  1.00 25.53    B   C
ATOM  3335  CD1 LEU B 170     -3.138  77.463  27.146  1.00 26.01    B   C
ATOM  3336  CD2 LEU B 170     -4.242  75.652  28.503  1.00 26.09    B   C
ATOM  3337  C   LEU B 170     -5.772  74.057  24.644  1.00 25.77    B   C
ATOM  3338  O   LEU B 170     -5.436  74.103  23.453  1.00 26.97    B   O
ATOM  3339  N   GLU B 171     -7.033  73.952  25.037  1.00 27.92    B   N
ATOM  3340  CA  GLU B 171     -8.117  73.860  24.078  1.00 30.46    B   C
ATOM  3341  CB  GLU B 171     -9.035  72.693  24.435  1.00 34.23    B   C
ATOM  3342  CG  GLU B 171     -8.408  71.310  24.268  1.00 36.53    B   C
ATOM  3343  CD  GLU B 171     -7.963  71.029  22.844  1.00 38.06    B   C
ATOM  3344  OE1 GLU B 171     -8.773  71.218  21.911  1.00 38.60    B   O
ATOM  3345  OE2 GLU B 171     -6.800  70.614  22.659  1.00 38.27    B   O
ATOM  3346  C   GLU B 171     -8.903  75.155  24.104  1.00 30.56    B   C
ATOM  3347  O   GLU B 171     -9.477  75.560  23.093  1.00 33.13    B   O
ATOM  3348  N   ILE B 172     -8.922  75.801  25.265  1.00 27.64    B   N
ATOM  3349  CA  ILE B 172     -9.627  77.060  25.428  1.00 26.46    B   C
ATOM  3350  CB  ILE B 172    -10.239  77.179  26.838  1.00 26.68    B   C
ATOM  3351  CG2 ILE B 172    -10.916  78.534  26.994  1.00 26.23    B   C
ATOM  3352  CG1 ILE B 172    -11.246  76.050  27.071  1.00 27.08    B   C
ATOM  3353  CD1 ILE B 172    -11.899  76.085  28.443  1.00 27.76    B   C
ATOM  3354  C   ILE B 172     -8.670  78.225  25.218  1.00 26.74    B   C
ATOM  3355  O   ILE B 172     -7.604  78.284  25.833  1.00 24.89    B   O
ATOM  3356  N   LEU B 173     -9.055  79.148  24.343  1.00 25.65    B   N
ATOM  3357  CA  LEU B 173     -8.245  80.328  24.061  1.00 25.77    B   C
ATOM  3358  CB  LEU B 173     -8.564  80.853  22.659  1.00 28.20    B   C
ATOM  3359  CG  LEU B 173     -7.682  81.962  22.082  1.00 29.17    B   C
ATOM  3360  CD1 LEU B 173     -6.227  81.521  22.081  1.00 31.35    B   C
ATOM  3361  CD2 LEU B 173     -8.144  82.281  20.661  1.00 29.98    B   C
ATOM  3362  C   LEU B 173     -8.585  81.387  25.111  1.00 24.69    B   C
ATOM  3363  O   LEU B 173     -9.720  81.852  25.188  1.00 26.80    B   O
ATOM  3364  N   PRO B 174     -7.606  81.780  25.939  1.00 21.86    B   N
ATOM  3365  CD  PRO B 174     -6.227  81.269  26.032  1.00 20.12    B   C
ATOM  3366  CA  PRO B 174     -7.857  82.786  26.973  1.00 21.00    B   C
ATOM  3367  CB  PRO B 174     -6.629  82.663  27.873  1.00 20.86    B   C
ATOM  3368  CG  PRO B 174     -5.553  82.313  26.900  1.00 20.88    B   C
ATOM  3369  C   PRO B 174     -8.058  84.215  26.481  1.00 21.07    B   C
ATOM  3370  O   PRO B 174     -7.442  84.652  25.510  1.00 20.92    B   O
ATOM  3371  N   GLU B 175     -8.941  84.932  27.163  1.00 20.88    B   N
ATOM  3372  CA  GLU B 175     -9.210  86.325  26.849  1.00 20.49    B   C
ATOM  3373  CB  GLU B 175    -10.714  86.599  26.886  1.00 22.18    B   C
ATOM  3374  CG  GLU B 175    -11.414  86.262  25.584  1.00 24.72    B   C
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Figure 4HHH

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ATOM  3375 CD  GLU B 175    -12.914  86.445  25.662  1.00 27.87      B   C
ATOM  3376 OE1 GLU B 175    -13.362  87.355  26.386  1.00 29.73,     B   O
ATOM  3377 OE2 GLU B 175    -13.643  85.686  24.989  1.00 30.38      B   O
ATOM  3378 C   GLU B 175     -8.492  87.110  27.932  1.00 19.76      B   C
ATOM  3379 O   GLU B 175     -8.151  88.278  27.760  1.00 19.06      B   O
ATOM  3380 N   VAL B 176     -8.249  86.429  29.047  1.00 18.72      B   N
ATOM  3381 CA  VAL B 176     -7.561  87.013  30.187  1.00 18.26      B   C
ATOM  3382 CB  VAL B 176     -8.542  87.366  31.329  1.00 19.04      B   C
ATOM  3383 CG1 VAL B 176     -7.792  88.005  32.473  1.00 17.96      B   C
ATOM  3384 CG2 VAL B 176     -9.627  88.307  30.819  1.00 19.77      B   C
ATOM  3385 C   VAL B 176     -6.566  85.994  30.728  1.00 18.77      B   C
ATOM  3386 O   VAL B 176     -6.909  84.830  30.936  1.00 18.44      B   O
ATOM  3387 N   ILE B 177     -5.337  86.438  30.955  1.00 15.78      B   N
ATOM  3388 CA  ILE B 177     -4.302  85.564  31.485  1.00 15.67      B   C
ATOM  3389 CB  ILE B 177     -3.149  85.366  30.479  1.00 16.57      B   C
ATOM  3390 CG2 ILE B 177     -2.076  84.471  31.092  1.00 15.73      B   C
ATOM  3391 CG1 ILE B 177     -3.679  84.754  29.184  1.00 17.67      B   C
ATOM  3392 CD1 ILE B 177     -2.639  84.634  28.094  1.00 16.12      B   C
ATOM  3393 C   ILE B 177     -3.730  86.191  32.746  1.00 15.83      B   C
ATOM  3394 O   ILE B 177     -3.319  87.356  32.742  1.00 15.47      B   O
ATOM  3395 N   ILE B 178     -3.721  85.427  33.832  1.00 15.84      B   N
ATOM  3396 CA  ILE B 178     -3.178  85.932  35.080  1.00 15.63      B   C
ATOM  3397 CB  ILE B 178     -3.958  85.402  36.314  1.00 16.93      B   C
ATOM  3398 CG2 ILE B 178     -3.370  85.986  37.589  1.00 15.87      B   C
ATOM  3399 CG1 ILE B 178     -5.432  85.807  36.228  1.00 18.02      B   C
ATOM  3400 CD1 ILE B 178     -6.267  85.341  37.422  1.00 17.46      B   C
ATOM  3401 C   ILE B 178     -1.724  85.486  35.190  1.00 14.02      B   C
ATOM  3402 O   ILE B 178     -1.416  84.300  35.089  1.00 13.65      B   O
ATOM  3403 N   LEU B 179     -0.833  86.449  35.376  1.00 14.12      B   N
ATOM  3404 CA  LEU B 179      0.589  86.150  35.525  1.00 14.34      B   C
ATOM  3405 CB  LEU B 179      1.428  87.340  35.053  1.00 15.34      B   C
ATOM  3406 CG  LEU B 179      1.169  87.783  33.610  1.00 16.04      B   C
ATOM  3407 CD1 LEU B 179      1.942  89.073  33.332  1.00 18.24      B   C
ATOM  3408 CD2 LEU B 179      1.574  86.680  32.636  1.00 16.26      B   C
ATOM  3409 C   LEU B 179      0.783  85.915  37.021  1.00 14.01      B   C
ATOM  3410 O   LEU B 179      1.391  86.727  37.719  1.00 13.42      B   O
ATOM  3411 N   GLY B 180      0.252  84.790  37.493  1.00 13.50      B   N
ATOM  3412 CA  GLY B 180      0.310  84.448  38.906  1.00 13.79      B   C
ATOM  3413 C   GLY B 180      1.632  83.927  39.417  1.00 12.30      B   C
ATOM  3414 O   GLY B 180      1.681  82.902  40.093  1.00 14.02      B   O
ATOM  3415 N   CYS B 181      2.702  84.647  39.093  1.00 13.12      B   N
ATOM  3416 CA  CYS B 181      4.048  84.295  39.518  1.00 11.26      B   C
ATOM  3417 CB  CYS B 181      4.591  83.150  38.667  1.00 11.52      B   C
ATOM  3418 SG  CYS B 181      6.279  82.671  39.091  1.00 14.29      B   S
ATOM  3419 C   CYS B 181      4.927  85.532  39.348  1.00 11.67      B   C
ATOM  3420 O   CYS B 181      4.837  86.226  38.336  1.00 10.15      B   O
ATOM  3421 N   THR B 182      5.770  85.796  40.342  1.00 10.95      B   N
ATOM  3422 CA  THR B 182      6.671  86.950  40.329  1.00 11.68      B   C
ATOM  3423 CB  THR B 182      7.654  86.902  41.517  1.00 12.29      B   C
ATOM  3424 OG1 THR B 182      8.306  85.623  41.546  1.00  8.82      B   O
ATOM  3425 CG2 THR B 182      6.918  87.133  42.832  1.00 13.05      B   C
ATOM  3426 C   THR B 182      7.511  87.085  39.068  1.00 12.00      B   C
ATOM  3427 O   THR B 182      7.775  88.190  38.604  1.00 11.14      B   O
ATOM  3428 N   HIS B 183      7.927  85.953  38.516  1.00 11.51      B   N
ATOM  3429 CA  HIS B 183      8.782  85.934  37.333  1.00 12.53      B   C
ATOM  3430 CB  HIS B 183      9.490  84.577  37.250  1.00 12.11      B   C
ATOM  3431 CG  HIS B 183     10.413  84.301  38.396  1.00 12.62      B   C
ATOM  3432 CD2 HIS B 183     11.662  83.774  38.425  1.00 14.37      B   C
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Figure 4III

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ATOM  3433 ND1 HIS B 183     10.074  84.558  39.708  1.00 12.87    B   N
ATOM  3434 CE1 HIS B 183     11.076  84.206  40.495  1.00 11.92    B   C
ATOM  3435 NE2 HIS B 183     12.051  83.728  39.741  1.00 12.64    B   N
ATOM  3436 C   HIS B 183     8.113  86.202  35.990  1.00 13.70    B   C
ATOM  3437 O   HIS B 183     8.735  86.757  35.082  1.00 14.63    B   O
ATOM  3438 N   PHE B 184     6.846  85.822  35.866  1.00 14.67    B   N
ATOM  3439 CA  PHE B 184     6.134  85.945  34.595  1.00 13.80    B   C
ATOM  3440 CB  PHE B 184     4.751  85.298  34.731  1.00 14.23    B   C
ATOM  3441 CG  PHE B 184     4.809  83.829  35.102  1.00 13.65    B   C
ATOM  3442 CD1 PHE B 184     3.646  83.084  35.240  1.00 16.74    B   C
ATOM  3443 CD2 PHE B 184     6.035  83.207  35.355  1.00 14.92    B   C
ATOM  3444 CE1 PHE B 184     3.698  81.743  35.631  1.00 13.35    B   C
ATOM  3445 CE2 PHE B 184     6.097  81.866  35.746  1.00 14.40    B   C
ATOM  3446 CZ  PHE B 184     4.923  81.136  35.884  1.00 13.35    B   C
ATOM  3447 C   PHE B 184     6.049  87.314  33.921  1.00 13.82    B   C
ATOM  3448 O   PHE B 184     5.991  87.391  32.691  1.00 13.30    B   O
ATOM  3449 N   PRO B 185     6.032  88.409  34.697  1.00 13.55    B   N
ATOM  3450 CD  PRO B 185     5.786  88.577  36.143  1.00 14.61    B   C
ATOM  3451 CA  PRO B 185     5.966  89.701  34.008  1.00 14.00    B   C
ATOM  3452 CB  PRO B 185     5.964  90.702  35.158  1.00 15.55    B   C
ATOM  3453 CG  PRO B 185     5.186  89.971  36.210  1.00 16.68    B   C
ATOM  3454 C   PRO B 185     7.158  89.907  33.063  1.00 14.41    B   C
ATOM  3455 O   PRO B 185     7.057  90.640  32.076  1.00 14.66    B   O
ATOM  3456 N   LEU B 186     8.285  89.257  33.355  1.00 13.60    B   N
ATOM  3457 CA  LEU B 186     9.462  89.410  32.503  1.00 14.78    B   C
ATOM  3458 CB  LEU B 186     10.707  88.844  33.185  1.00 16.45    B   C
ATOM  3459 CG  LEU B 186     11.268  89.716  34.312  1.00 17.76    B   C
ATOM  3460 CD1 LEU B 186     12.601  89.149  34.788  1.00 18.57    B   C
ATOM  3461 CD2 LEU B 186     11.454  91.145  33.800  1.00 19.96    B   C
ATOM  3462 C   LEU B 186     9.299  88.796  31.115  1.00 14.26    B   C
ATOM  3463 O   LEU B 186     10.105  89.060  30.219  1.00 13.67    B   O
ATOM  3464 N   ILE B 187     8.271  87.973  30.933  1.00 13.72    B   N
ATOM  3465 CA  ILE B 187     8.007  87.391  29.616  1.00 14.52    B   C
ATOM  3466 CB  ILE B 187     8.252  85.852  29.567  1.00 16.13    B   C
ATOM  3467 CG2 ILE B 187     9.734  85.563  29.730  1.00 15.11    B   C
ATOM  3468 CG1 ILE B 187     7.418  85.134  30.630  1.00 14.95    B   C
ATOM  3469 CD1 ILE B 187     7.386  83.616  30.452  1.00 18.91    B   C
ATOM  3470 C   ILE B 187     6.559  87.681  29.216  1.00 15.97    B   C
ATOM  3471 O   ILE B 187     5.970  86.973  28.399  1.00 14.41    B   O
ATOM  3472 N   ALA B 188     6.003  88.742  29.790  1.00 14.30    B   N
ATOM  3473 CA  ALA B 188     4.623  89.138  29.511  1.00 16.72    B   C
ATOM  3474 CB  ALA B 188     4.261  90.381  30.318  1.00 17.73    B   C
ATOM  3475 C   ALA B 188     4.386  89.386  28.021  1.00 17.75    B   C
ATOM  3476 O   ALA B 188     3.473  88.806  27.437  1.00 15.55    B   O
ATOM  3477 N   GLN B 189     5.208  90.232  27.404  1.00 18.64    B   N
ATOM  3478 CA  GLN B 189     5.045  90.521  25.979  1.00 20.60    B   C
ATOM  3479 CB  GLN B 189     5.977  91.668  25.553  1.00 24.25    B   C
ATOM  3480 CG  GLN B 189     7.448  91.297  25.369  1.00 34.75    B   C
ATOM  3481 CD  GLN B 189     8.385  92.508  25.450  1.00 39.99    B   C
ATOM  3482 OE1 GLN B 189     7.963  93.653  25.263  1.00 43.74    B   O
ATOM  3483 NE2 GLN B 189     9.663  92.254  25.720  1.00 40.19    B   N
ATOM  3484 C   GLN B 189     5.279  89.273  25.111  1.00 17.97    B   C
ATOM  3485 O   GLN B 189     4.729  89.163  24.015  1.00 14.32    B   O
ATOM  3486 N   LYS B 190     6.078  88.329  25.606  1.00 17.40    B   N
ATOM  3487 CA  LYS B 190     6.341  87.097  24.859  1.00 16.80    B   C
ATOM  3488 CB  LYS B 190     7.567  86.374  25.421  1.00 18.22    B   C
ATOM  3489 CG  LYS B 190     8.878  87.117  25.218  1.00 21.88    B   C
ATOM  3490 CD  LYS B 190     9.211  87.269  23.740  1.00 25.45    B   C
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Figure 4JJJ

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ATOM  3491 CE  LYS B 190     10.416  88.179  23.543  1.00 29.36    B   C
ATOM  3492 NZ  LYS B 190     10.790  88.298  22.110  1.00 29.28    B   N
ATOM  3493 C   LYS B 190      5.123  86.176  24.920  1.00 16.76    B   C
ATOM  3494 O   LYS B 190      4.775  85.521  23.934  1.00 15.72    B   O
ATOM  3495 N   ILE B 191      4.484  86.118  26.085  1.00 17.36    B   N
ATOM  3496 CA  ILE B 191      3.293  85.293  26.250  1.00 16.65    B   C
ATOM  3497 CB  ILE B 191      2.835  85.283  27.722  1.00 16.29    B   C
ATOM  3498 CG2 ILE B 191      1.429  84.706  27.837  1.00 15.90    B   C
ATOM  3499 CG1 ILE B 191      3.827  84.472  28.561  1.00 14.41    B   C
ATOM  3500 CD1 ILE B 191      3.575  84.556  30.065  1.00 15.15    B   C
ATOM  3501 C   ILE B 191      2.206  85.902  25.371  1.00 17.73    B   C
ATOM  3502 O   ILE B 191      1.431  85.201  24.730  1.00 17.39    B   O
ATOM  3503 N   GLU B 192      2.174  87.227  25.343  1.00 19.90    B   N
ATOM  3504 CA  GLU B 192      1.206  87.955  24.545  1.00 20.35    B   C
ATOM  3505 CB  GLU B 192      1.368  89.452  24.811  1.00 22.52    B   C
ATOM  3506 CG  GLU B 192      0.186  90.301  24.426  1.00 31.49    B   C
ATOM  3507 CD  GLU B 192      0.310  91.705  24.981  1.00 36.51    B   C
ATOM  3508 OE1 GLU B 192      0.342  91.845  26.223  1.00 39.33    B   O
ATOM  3509 OE2 GLU B 192      0.384  92.660  24.179  1.00 38.77    B   O
ATOM  3510 C   GLU B 192      1.468  87.638  23.077  1.00 18.85    B   C
ATOM  3511 O   GLU B 192      0.553  87.274  22.327  1.00 18.00    B   O
ATOM  3512 N   GLY B 193      2.733  87.764  22.685  1.00 19.26    B   N
ATOM  3513 CA  GLY B 193      3.134  87.497  21.319  1.00 16.37    B   C
ATOM  3514 C   GLY B 193      2.843  86.078  20.880  1.00 17.40    B   C
ATOM  3515 O   GLY B 193      2.580  85.832  19.700  1.00 19.53    B   O
ATOM  3516 N   TYR B 194      2.892  85.138  21.819  1.00 15.60    B   N
ATOM  3517 CA  TYR B 194      2.621  83.740  21.494  1.00 16.39    B   C
ATOM  3518 CB  TYR B 194      2.829  82.845  22.715  1.00 16.47    B   C
ATOM  3519 CG  TYR B 194      2.502  81.386  22.452  1.00 15.75    B   C
ATOM  3520 CD1 TYR B 194      3.470  80.515  21.964  1.00 17.79    B   C
ATOM  3521 CE1 TYR B 194      3.171  79.178  21.698  1.00 18.26    B   C
ATOM  3522 CD2 TYR B 194      1.216  80.887  22.669  1.00 15.15    B   C
ATOM  3523 CE2 TYR B 194      0.904  79.551  22.403  1.00 16.44    B   C
ATOM  3524 CZ  TYR B 194      1.890  78.703  21.920  1.00 15.60    B   C
ATOM  3525 OH  TYR B 194      1.614  77.379  21.671  1.00 17.72    B   O
ATOM  3526 C   TYR B 194      1.189  83.551  21.003  1.00 16.01    B   C
ATOM  3527 O   TYR B 194      0.966  82.985  19.940  1.00 17.33    B   O
ATOM  3528 N   PHE B 195      0.218  84.011  21.785  1.00 17.37    B   N
ATOM  3529 CA  PHE B 195     -1.177  83.851  21.390  1.00 19.84    B   C
ATOM  3530 CB  PHE B 195     -2.108  84.174  22.563  1.00 20.48    B   C
ATOM  3531 CG  PHE B 195     -2.057  83.146  23.659  1.00 21.18    B   C
ATOM  3532 CD1 PHE B 195     -1.166  83.281  24.720  1.00 20.24    B   C
ATOM  3533 CD2 PHE B 195     -2.847  82.002  23.590  1.00 20.40    B   C
ATOM  3534 CE1 PHE B 195     -1.061  82.289  25.692  1.00 18.52    B   C
ATOM  3535 CE2 PHE B 195     -2.748  81.004  24.558  1.00 21.83    B   C
ATOM  3536 CZ  PHE B 195     -1.853  81.149  25.609  1.00 18.80    B   C
ATOM  3537 C   PHE B 195     -1.549  84.675  20.168  1.00 21.22    B   C
ATOM  3538 O   PHE B 195     -2.381  84.260  19.364  1.00 23.42    B   O
ATOM  3539 N   MET B 196     -0.920  85.835  20.018  1.00 20.91    B   N
ATOM  3540 CA  MET B 196     -1.191  86.691  18.874  1.00 22.63    B   C
ATOM  3541 CB  MET B 196     -0.632  88.096  19.110  1.00 21.19    B   C
ATOM  3542 CG  MET B 196     -1.454  88.939  20.066  1.00 21.47    B   C
ATOM  3543 SD  MET B 196     -3.106  89.333  19.420  1.00 22.89    B   S
ATOM  3544 CE  MET B 196     -2.734  90.738  18.369  1.00 25.90    B   C
ATOM  3545 C   MET B 196     -0.574  86.098  17.616  1.00 22.76    B   C
ATOM  3546 O   MET B 196     -1.034  86.365  16.510  1.00 22.32    B   O
ATOM  3547 N   GLY B 197      0.462  85.284  17.788  1.00 23.35    B   N
ATOM  3548 CA  GLY B 197      1.117  84.682  16.644  1.00 23.78    B   C
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Figure 4KKK

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ATOM  3549  C   GLY B 197      0.612  83.294  16.308  1.00 26.07      B   C
ATOM  3550  O   GLY B 197      0.757  82.836  15.178  1.00 27.06      B   O
ATOM  3551  N   HIS B 198      0.011  82.618  17.280  1.00 24.62      B   N
ATOM  3552  CA  HIS B 198     -0.489  81.270  17.052  1.00 25.26      B   C
ATOM  3553  CB  HIS B 198     -0.143  80.393  18.250  1.00 24.79      B   C
ATOM  3554  CG  HIS B 198      1.318  80.087  18.358  1.00 27.65      B   C
ATOM  3555  CD2 HIS B 198      2.369  80.867  18.706  1.00 27.06      B   C
ATOM  3556  ND1 HIS B 198      1.847  78.858  18.026  1.00 29.54      B   N
ATOM  3557  CE1 HIS B 198      3.161  78.896  18.162  1.00 28.74      B   C
ATOM  3558  NE2 HIS B 198      3.503  80.104  18.572  1.00 27.31      B   N
ATOM  3559  C   HIS B 198     -1.982  81.189  16.742  1.00 25.16      B   C
ATOM  3560  O   HIS B 198     -2.470  80.160  16.274  1.00 25.84      B   O
ATOM  3561  N   PHE B 199     -2.701  82.274  17.002  1.00 23.99      B   N
ATOM  3562  CA  PHE B 199     -4.134  82.323  16.731  1.00 25.24      B   C
ATOM  3563  CB  PHE B 199     -4.939  82.150  18.021  1.00 25.35      B   C
ATOM  3564  CG  PHE B 199     -4.641  80.875  18.754  1.00 25.83      B   C
ATOM  3565  CD1 PHE B 199     -3.499  80.763  19.543  1.00 25.81      B   C
ATOM  3566  CD2 PHE B 199     -5.486  79.776  18.634  1.00 26.63      B   C
ATOM  3567  CE1 PHE B 199     -3.202  79.571  20.204  1.00 25.90      B   C
ATOM  3568  CE2 PHE B 199     -5.200  78.574  19.292  1.00 27.07      B   C
ATOM  3569  CZ  PHE B 199     -4.053  78.476  20.078  1.00 25.59      B   C
ATOM  3570  C   PHE B 199     -4.488  83.658  16.085  1.00 25.45      B   C
ATOM  3571  O   PHE B 199     -3.741  84.633  16.202  1.00 26.05      B   O
ATOM  3572  N   ALA B 200     -5.624  83.698  15.397  1.00 25.36      B   N
ATOM  3573  CA  ALA B 200     -6.066  84.926  14.744  1.00 26.49      B   C
ATOM  3574  CB  ALA B 200     -6.945  84.592  13.543  1.00 27.04      B   C
ATOM  3575  C   ALA B 200     -6.842  85.770  15.748  1.00 25.75      B   C
ATOM  3576  O   ALA B 200     -8.035  85.555  15.951  1.00 27.07      B   O
ATOM  3577  N   LEU B 201     -6.162  86.723  16.380  1.00 26.03      B   N
ATOM  3578  CA  LEU B 201     -6.801  87.588  17.371  1.00 25.45      B   C
ATOM  3579  CB  LEU B 201     -6.206  87.345  18.762  1.00 26.37      B   C
ATOM  3580  CG  LEU B 201     -6.409  85.971  19.404  1.00 27.87      B   C
ATOM  3581  CD1 LEU B 201     -5.727  85.944  20.768  1.00 27.55      B   C
ATOM  3582  CD2 LEU B 201     -7.895  85.681  19.539  1.00 28.11      B   C
ATOM  3583  C   LEU B 201     -6.668  89.069  17.041  1.00 24.86      B   C
ATOM  3584  O   LEU B 201     -5.571  89.565  16.801  1.00 25.77      B   O
ATOM  3585  N   PRO B 202     -7.792  89.795  17.036  1.00 25.07      B   N
ATOM  3586  CD  PRO B 202     -9.159  89.302  17.284  1.00 27.27      B   C
ATOM  3587  CA  PRO B 202     -7.801  91.229  16.739  1.00 27.30      B   C
ATOM  3588  CB  PRO B 202     -9.286  91.530  16.571  1.00 26.61      B   C
ATOM  3589  CG  PRO B 202     -9.919  90.581  17.541  1.00 28.74      B   C
ATOM  3590  C   PRO B 202     -7.162  92.024  17.878  1.00 28.85      B   C
ATOM  3591  O   PRO B 202     -6.625  93.111  17.676  1.00 31.54      B   O
ATOM  3592  N   THR B 203     -7.228  91.467  19.080  1.00 29.83      B   N
ATOM  3593  CA  THR B 203     -6.649  92.104  20.253  1.00 30.73      B   C
ATOM  3594  CB  THR B 203     -7.717  92.910  21.029  1.00 32.69      B   C
ATOM  3595  OG1 THR B 203     -7.113  93.535  22.168  1.00 38.76      B   O
ATOM  3596  CG2 THR B 203     -8.854  92.009  21.478  1.00 34.49      B   C
ATOM  3597  C   THR B 203     -6.057  91.009  21.142  1.00 30.11      B   C
ATOM  3598  O   THR B 203     -6.632  89.929  21.281  1.00 29.77      B   O
ATOM  3599  N   PRO B 204     -4.888  91.271  21.746  1.00 28.28      B   N
ATOM  3600  CD  PRO B 204     -4.105  92.519  21.714  1.00 29.99      B   C
ATOM  3601  CA  PRO B 204     -4.249  90.278  22.608  1.00 25.72      B   C
ATOM  3602  CB  PRO B 204     -2.871  90.878  22.851  1.00 27.64      B   C
ATOM  3603  CG  PRO B 204     -3.170  92.344  22.895  1.00 30.54      B   C
ATOM  3604  C   PRO B 204     -5.007  90.034  23.906  1.00 22.99      B   C
ATOM  3605  O   PRO B 204     -5.829  90.847  24.322  1.00 21.45      B   O
ATOM  3606  N   PRO B 205     -4.754  88.888  24.550  1.00 23.17      B   N
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Figure 4LLL

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ATOM  3607 CD  PRO B 205     -3.967  87.734  24.079  1.00 22.14    B   C
ATOM  3608 CA  PRO B 205     -5.435  88.579  25.812  1.00 21.71    B   C
ATOM  3609 CB  PRO B 205     -4.930  87.177  26.145  1.00 20.02    B   C
ATOM  3610 CG  PRO B 205     -4.640  86.587  24.791  1.00 24.28    B   C
ATOM  3611 C   PRO B 205     -5.013  89.592  26.870  1.00 20.42    B   C
ATOM  3612 O   PRO B 205     -3.884  90.081  26.855  1.00 20.68    B   O
ATOM  3613 N   LEU B 206     -5.920  89.912  27.781  1.00 19.56    B   N
ATOM  3614 CA  LEU B 206     -5.614  90.852  28.844  1.00 18.19    B   C
ATOM  3615 CB  LEU B 206     -6.903  91.341  29.506  1.00 19.98    B   C
ATOM  3616 CG  LEU B 206     -6.733  92.187  30.772  1.00 20.16    B   C
ATOM  3617 CD1 LEU B 206     -6.025  93.490  30.435  1.00 20.32    B   C
ATOM  3618 CD2 LEU B 206     -8.097  92.461  31.383  1.00 21.77    B   C
ATOM  3619 C   LEU B 206     -4.748  90.152  29.887  1.00 19.09    B   C
ATOM  3620 O   LEU B 206     -5.155  89.137  30.460  1.00 16.01    B   O
ATOM  3621 N   LEU B 207     -3.554  90.682  30.130  1.00 17.87    B   N
ATOM  3622 CA  LEU B 207     -2.673  90.086  31.128  1.00 19.96    B   C
ATOM  3623 CB  LEU B 207     -1.204  90.137  30.683  1.00 20.75    B   C
ATOM  3624 CG  LEU B 207     -0.775  89.375  29.427  1.00 23.64    B   C
ATOM  3625 CD1 LEU B 207      0.754  89.247  29.409  1.00 24.69    B   C
ATOM  3626 CD2 LEU B 207     -1.402  88.003  29.411  1.00 25.49    B   C
ATOM  3627 C   LEU B 207     -2.822  90.826  32.450  1.00 18.55    B   C
ATOM  3628 O   LEU B 207     -2.846  92.056  32.489  1.00 19.17    B   O
ATOM  3629 N   ILE B 208     -2.925  90.067  33.534  1.00 17.96    B   N
ATOM  3630 CA  ILE B 208     -3.064  90.645  34.860  1.00 17.50    B   C
ATOM  3631 CB  ILE B 208     -4.118  89.878  35.685  1.00 17.43    B   C
ATOM  3632 CG2 ILE B 208     -4.243  90.491  37.077  1.00 18.18    B   C
ATOM  3633 CG1 ILE B 208     -5.459  89.892  34.943  1.00 18.45    B   C
ATOM  3634 CD1 ILE B 208     -6.012  91.289  34.699  1.00 14.50    B   C
ATOM  3635 C   ILE B 208     -1.719  90.585  35.575  1.00 16.82    B   C
ATOM  3636 O   ILE B 208     -1.164  89.508  35.780  1.00 15.89    B   O
ATOM  3637 N   HIS B 209     -1.213  91.756  35.950  1.00 17.14    B   N
ATOM  3638 CA  HIS B 209      0.074  91.899  36.632  1.00 18.16    B   C
ATOM  3639 CB  HIS B 209      0.745  93.175  36.106  1.00 18.91    B   C
ATOM  3640 CG  HIS B 209      2.193  93.306  36.457  1.00 20.99    B   C
ATOM  3641 CD2 HIS B 209      3.306  93.162  35.699  1.00 19.36    B   C
ATOM  3642 ND1 HIS B 209      2.629  93.657  37.716  1.00 22.36    B   N
ATOM  3643 CE1 HIS B 209      3.949  93.725  37.718  1.00 21.52    B   C
ATOM  3644 NE2 HIS B 209      4.384  93.429  36.506  1.00 15.94    B   N
ATOM  3645 C   HIS B 209     -0.149  91.980  38.150  1.00 17.31    B   C
ATOM  3646 O   HIS B 209     -0.909  92.826  38.621  1.00 17.80    B   O
ATOM  3647 N   SER B 210      0.513  91.104  38.908  1.00 15.90    B   N
ATOM  3648 CA  SER B 210      0.361  91.070  40.366  1.00 18.09    B   C
ATOM  3649 CB  SER B 210      1.187  89.931  40.975  1.00 15.92    B   C
ATOM  3650 OG  SER B 210      0.783  88.671  40.475  1.00 17.30    B   O
ATOM  3651 C   SER B 210      0.762  92.368  41.048  1.00 18.89    B   C
ATOM  3652 O   SER B 210      0.146  92.783  42.036  1.00 18.64    B   O
ATOM  3653 N   GLY B 211      1.806  92.999  40.527  1.00 18.49    B   N
ATOM  3654 CA  GLY B 211      2.276  94.241  41.105  1.00 17.93    B   C
ATOM  3655 C   GLY B 211      1.300  95.384  40.929  1.00 18.65    B   C
ATOM  3656 O   GLY B 211      0.988  96.088  41.888  1.00 18.89    B   O
ATOM  3657 N   ASP B 212      0.821  95.585  39.708  1.00 17.89    B   N
ATOM  3658 CA  ASP B 212     -0.122  96.666  39.454  1.00 19.78    B   C
ATOM  3659 CB  ASP B 212     -0.441  96.776  37.959  1.00 21.36    B   C
ATOM  3660 CG  ASP B 212      0.789  97.074  37.119  1.00 25.55    B   C
ATOM  3661 OD1 ASP B 212      1.588  97.954  37.509  1.00 24.93    B   O
ATOM  3662 OD2 ASP B 212      0.948  96.432  36.059  1.00 27.71    B   O
ATOM  3663 C   ASP B 212     -1.414  96.441  40.227  1.00 18.76    B   C
ATOM  3664 O   ASP B 212     -2.025  97.389  40.712  1.00 19.27    B   O
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Figure 4MMM

ATOM 3665 N ALA B 213 -1.825 95.182 40.344 1.00 19.86 B N
ATOM 3666 CA ALA B 213 -3.055 94.847 41.054 1.00 17.54 B C
ATOM 3667 CB ALA B 213 -3.378 93.372 40.876 1.00 17.05 B C
ATOM 3668 C ALA B 213 -2.959 95.183 42.539 1.00 19.06 B C
ATOM 3669 O ALA B 213 -3.901 95.725 43.120 1.00 16.90 B O
ATOM 3670 N ILE B 214 -1.823 94.876 43.158 1.00 15.97 B N
ATOM 3671 CA ILE B 214 -1.678 95.162 44.577 1.00 16.41 B C
ATOM 3672 CB ILE B 214 -0.503 94.357 45.206 1.00 17.51 B C
ATOM 3673 CG2 ILE B 214 0.841 94.960 44.809 1.00 16.99 B C
ATOM 3674 CG1 ILE B 214 -0.639 94.359 46.733 1.00 17.48 B C
ATOM 3675 CD1 ILE B 214 0.283 93.366 47.436 1.00 20.67 B C
ATOM 3676 C ILE B 214 -1.516 96.656 44.864 1.00 16.49 B C
ATOM 3677 O ILE B 214 -1.933 97.133 45.917 1.00 16.10 B O
ATOM 3678 N VAL B 215 -0.927 97.403 43.933 1.00 16.36 B N
ATOM 3679 CA VAL B 215 -0.772 98.841 44.139 1.00 17.16 B C
ATOM 3680 CB VAL B 215 -0.016 99.509 42.964 1.00 19.48 B C
ATOM 3681 CG1 VAL B 215 -0.179 101.017 43.027 1.00 17.77 B C
ATOM 3682 CG2 VAL B 215 1.470 99.147 43.022 1.00 17.10 B C
ATOM 3683 C VAL B 215 -2.161 99.471 44.259 1.00 18.05 B C
ATOM 3684 O VAL B 215 -2.417 100.282 45.153 1.00 17.39 B O
ATOM 3685 N GLU B 216 -3.054 99.089 43.354 1.00 19.67 B N
ATOM 3686 CA GLU B 216 -4.411 99.617 43.357 1.00 21.54 B C
ATOM 3687 CB GLU B 216 -5.188 99.059 42.166 1.00 23.84 B C
ATOM 3688 CG GLU B 216 -4.815 99.727 40.853 1.00 26.87 B C
ATOM 3689 CD GLU B 216 -5.388 99.014 39.648 1.00 30.91 B C
ATOM 3690 OE1 GLU B 216 -5.399 99.623 38.558 1.00 34.30 B O
ATOM 3691 OE2 GLU B 216 -5.815 97.845 39.785 1.00 31.99 B O
ATOM 3692 C GLU B 216 -5.126 99.293 44.657 1.00 20.92 B C
ATOM 3693 O GLU B 216 -5.815 100.141 45.223 1.00 19.64 B O
ATOM 3694 N TYR B 217 -4.955 98.065 45.135 1.00 21.71 B N
ATOM 3695 CA TYR B 217 -5.583 97.649 46.386 1.00 21.99 B C
ATOM 3696 CB TYR B 217 -5.307 96.167 46.658 1.00 22.18 B C
ATOM 3697 CG TYR B 217 -5.831 95.693 47.995 1.00 20.53 B C
ATOM 3698 CD1 TYR B 217 -7.199 95.534 48.213 1.00 22.61 B C
ATOM 3699 CE1 TYR B 217 -7.692 95.113 49.456 1.00 20.09 B C
ATOM 3700 CD2 TYR B 217 -4.961 95.422 49.051 1.00 19.57 B C
ATOM 3701 CE2 TYR B 217 -5.440 95.002 50.293 1.00 19.82 B C
ATOM 3702 CZ TYR B 217 -6.807 94.849 50.488 1.00 20.38 B C
ATOM 3703 OH TYR B 217 -7.288 94.422 51.709 1.00 19.08 B O
ATOM 3704 C TYR B 217 -5.056 98.473 47.558 1.00 22.00 B C
ATOM 3705 O TYR B 217 -5.832 98.992 48.362 1.00 21.85 B O
ATOM 3706 N LEU B 218 -3.734 98.591 47.654 1.00 19.08 B N
ATOM 3707 CA LEU B 218 -3.113 99.341 48.740 1.00 19.40 B C
ATOM 3708 CB LEU B 218 -1.585 99.279 48.615 1.00 17.82 B C
ATOM 3709 CG LEU B 218 -0.941 97.888 48.742 1.00 18.28 B C
ATOM 3710 CD1 LEU B 218 0.541 97.968 48.389 1.00 15.96 B C
ATOM 3711 CD2 LEU B 218 -1.128 97.353 50.155 1.00 16.26 B C
ATOM 3712 C LEU B 218 -3.582 100.798 48.791 1.00 21.94 B C
ATOM 3713 O LEU B 218 -3.841 101.335 49.866 1.00 18.51 B O
ATOM 3714 N GLN B 219 -3.691 101.433 47.629 1.00 22.92 B N
ATOM 3715 CA GLN B 219 -4.139 102.822 47.562 1.00 24.80 B C
ATOM 3716 CB GLN B 219 -4.004 103.353 46.129 1.00 26.04 B C
ATOM 3717 CG GLN B 219 -2.577 103.325 45.592 1.00 28.25 B C
ATOM 3718 CD GLN B 219 -2.470 103.820 44.156 1.00 28.07 B C
ATOM 3719 OE1 GLN B 219 -3.166 103.334 43.262 1.00 25.98 B O
ATOM 3720 NE2 GLN B 219 -1.588 104.790 43.932 1.00 30.48 B N
ATOM 3721 C GLN B 219 -5.596 102.914 48.005 1.00 24.27 B C
ATOM 3722 O GLN B 219 -5.995 103.859 48.683 1.00 25.16 B O

Figure 4NNN

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ATOM  3723 N   GLN B 220    -6.375 101.912  47.620  1.00 24.30      B   N
ATOM  3724 CA  GLN B 220    -7.792 101.838  47.943  1.00 28.00      B   C
ATOM  3725 CB  GLN B 220    -8.410 100.663  47.184  1.00 31.02      B   C
ATOM  3726 CG  GLN B 220    -9.920 100.674  47.077  1.00 39.36      B   C
ATOM  3727 CD  GLN B 220   -10.411 101.639  46.020  1.00 44.14      B   C
ATOM  3728 OE1 GLN B 220   -10.260 102.854  46.154  1.00 47.44      B   O
ATOM  3729 NE2 GLN B 220   -10.995 101.101  44.954  1.00 47.51      B   N
ATOM  3730 C   GLN B 220    -8.013 101.635  49.444  1.00 29.46      B   C
ATOM  3731 O   GLN B 220    -8.553 102.499  50.137  1.00 28.33      B   O
ATOM  3732 N   LYS B 221    -7.570 100.477  49.927  1.00 29.84      B   N
ATOM  3733 CA  LYS B 221    -7.720 100.075  51.321  1.00 28.05      B   C
ATOM  3734 CB  LYS B 221    -7.249  98.626  51.477  1.00 29.20      B   C
ATOM  3735 CG  LYS B 221    -8.124  97.761  52.381  1.00 33.06      B   C
ATOM  3736 CD  LYS B 221    -8.114  98.242  53.817  1.00 34.46      B   C
ATOM  3737 CE  LYS B 221    -8.796  97.239  54.738  1.00 34.63      B   C
ATOM  3738 NZ  LYS B 221    -8.003  95.993  54.896  1.00 31.31      B   N
ATOM  3739 C   LYS B 221    -7.012 100.953  52.345  1.00 27.08      B   C
ATOM  3740 O   LYS B 221    -7.556 101.230  53.416  1.00 27.24      B   O
ATOM  3741 N   TYR B 222    -5.804 101.399  52.029  1.00 25.82      B   N
ATOM  3742 CA  TYR B 222    -5.052 102.212  52.973  1.00 27.04      B   C
ATOM  3743 CB  TYR B 222    -3.658 101.616  53.147  1.00 22.44      B   C
ATOM  3744 CG  TYR B 222    -3.708 100.166  53.576  1.00 22.86      B   C
ATOM  3745 CD1 TYR B 222    -4.156  99.815  54.854  1.00 19.32      B   C
ATOM  3746 CE1 TYR B 222    -4.258  98.484  55.243  1.00 19.44      B   C
ATOM  3747 CD2 TYR B 222    -3.357  99.134  52.694  1.00 20.72      B   C
ATOM  3748 CE2 TYR B 222    -3.456  97.792  53.078  1.00 19.21      B   C
ATOM  3749 CZ  TYR B 222    -3.909  97.482  54.351  1.00 19.82      B   C
ATOM  3750 OH  TYR B 222    -4.027  96.167  54.725  1.00 19.05      B   O
ATOM  3751 C   TYR B 222    -4.968 103.667  52.539  1.00 29.48      B   C
ATOM  3752 O   TYR B 222    -4.096 104.405  52.986  1.00 31.72      B   O
ATOM  3753 N   ALA B 223    -5.900 104.089  51.696  1.00 32.87      B   N
ATOM  3754 CA  ALA B 223    -5.895 105.466  51.201  1.00 36.60      B   C
ATOM  3755 CB  ALA B 223    -6.672 106.421  52.148  1.00 37.41      B   C
ATOM  3756 C   ALA B 223    -4.442 105.909  51.088  1.00 38.06      B   C
ATOM  3757 O   ALA B 223    -4.060 106.977  51.560  1.00 38.78      B   O
ATOM  3758 N   LEU B 224    -3.627 105.088  50.441  1.00 38.57      B   N
ATOM  3759 CA  LEU B 224    -2.215 105.403  50.264  1.00 38.61      B   C
ATOM  3760 CB  LEU B 224    -1.402 104.097  50.136  1.00 39.37      B   C
ATOM  3761 CG  LEU B 224    -1.183 103.355  51.466  1.00 39.96      B   C
ATOM  3762 CD1 LEU B 224    -0.057 102.350  51.297  1.00 39.16      B   C
ATOM  3763 CD2 LEU B 224    -0.818 104.336  52.585  1.00 41.79      B   C
ATOM  3764 C   LEU B 224    -1.949 106.306  49.064  1.00 38.91      B   C
ATOM  3765 O   LEU B 224    -2.714 106.190  48.105  1.00 38.22      B   O
ATOM  3766 OXT LEU B 224    -0.969 107.085  49.068  1.00 39.30      B   O
ATOM  3767 CB  PRO B 232    11.684 106.007  48.754  1.00 35.25      B   C
ATOM  3768 CG  PRO B 232    11.385 107.285  47.963  1.00 36.48      B   C
ATOM  3769 C   PRO B 232    13.583 105.559  50.328  1.00 32.21      B   C
ATOM  3770 O   PRO B 232    14.407 105.139  49.517  1.00 33.63      B   O
ATOM  3771 N   PRO B 232    13.132 107.820  49.423  1.00 34.70      B   N
ATOM  3772 CD  PRO B 232    12.673 108.108  48.053  1.00 35.80      B   C
ATOM  3773 CA  PRO B 232    12.514 106.559  49.903  1.00 34.68      B   C
ATOM  3774 N   LYS B 233    13.566 105.183  51.602  1.00 30.94      B   N
ATOM  3775 CA  LYS B 233    14.542 104.237  52.126  1.00 27.68      B   C
ATOM  3776 CB  LYS B 233    14.693 104.412  53.637  1.00 30.73      B   C
ATOM  3777 CG  LYS B 233    15.074 105.817  54.076  1.00 37.18      B   C
ATOM  3778 CD  LYS B 233    15.073 105.930  55.594  1.00 41.29      B   C
ATOM  3779 CE  LYS B 233    15.358 107.357  56.045  1.00 46.10      B   C
ATOM  3780 NZ  LYS B 233    15.389 107.476  57.535  1.00 49.46      B   N
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Figure 4OOO

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ATOM  3781  C   LYS B 233     14.115 102.805  51.823  1.00 25.78    B   C
ATOM  3782  O   LYS B 233     12.984 102.404  52.108  1.00 21.74    B   O
ATOM  3783  N   VAL B 234     15.027 102.041  51.238  1.00 23.23    B   N
ATOM  3784  CA  VAL B 234     14.755 100.652  50.902  1.00 22.01    B   C
ATOM  3785  CB  VAL B 234     14.425 100.486  49.403  1.00 22.47    B   C
ATOM  3786  CG1 VAL B 234     14.095  99.034  49.105  1.00 23.89    B   C
ATOM  3787  CG2 VAL B 234     13.267 101.386  49.015  1.00 24.31    B   C
ATOM  3788  C   VAL B 234     15.997  99.825  51.204  1.00 21.91    B   C
ATOM  3789  O   VAL B 234     17.083 100.121  50.702  1.00 19.49    B   O
ATOM  3790  N   GLU B 235     15.850  98.805  52.041  1.00 19.26    B   N
ATOM  3791  CA  GLU B 235     16.987  97.956  52.343  1.00 19.57    B   C
ATOM  3792  CB  GLU B 235     17.407  98.085  53.812  1.00 22.19    B   C
ATOM  3793  CG  GLU B 235     16.367  97.736  54.849  1.00 27.30    B   C
ATOM  3794  CD  GLU B 235     16.893  97.954  56.266  1.00 31.20    B   C
ATOM  3795  OE1 GLU B 235     17.214  99.113  56.617  1.00 30.91    B   O
ATOM  3796  OE2 GLU B 235     16.992  96.967  57.027  1.00 31.05    B   O
ATOM  3797  C   GLU B 235     16.667  96.513  51.979  1.00 17.90    B   C
ATOM  3798  O   GLU B 235     15.514  96.071  52.067  1.00 17.20    B   O
ATOM  3799  N   PHE B 236     17.694  95.797  51.538  1.00 15.16    B   N
ATOM  3800  CA  PHE B 236     17.540  94.417  51.121  1.00 14.57    B   C
ATOM  3801  CB  PHE B 236     18.080  94.240  49.702  1.00 13.24    B   C
ATOM  3802  CG  PHE B 236     17.406  95.123  48.695  1.00 14.78    B   C
ATOM  3803  CD1 PHE B 236     17.807  96.448  48.529  1.00 13.54    B   C
ATOM  3804  CD2 PHE B 236     16.338  94.647  47.944  1.00 13.10    B   C
ATOM  3805  CE1 PHE B 236     17.148  97.281  47.625  1.00 15.52    B   C
ATOM  3806  CE2 PHE B 236     15.676  95.471  47.043  1.00 11.79    B   C
ATOM  3807  CZ  PHE B 236     16.083  96.792  46.884  1.00 13.41    B   C
ATOM  3808  C   PHE B 236     18.206  93.432  52.055  1.00 14.79    B   C
ATOM  3809  O   PHE B 236     19.298  93.668  52.566  1.00 14.15    B   O
ATOM  3810  N   HIS B 237     17.519  92.319  52.270  1.00 13.68    B   N
ATOM  3811  CA  HIS B 237     17.993  91.266  53.147  1.00 11.28    B   C
ATOM  3812  CB  HIS B 237     17.235  91.319  54.466  1.00 12.27    B   C
ATOM  3813  CG  HIS B 237     17.437  92.597  55.219  1.00 14.02    B   C
ATOM  3814  CD2 HIS B 237     16.779  93.778  55.159  1.00 14.88    B   C
ATOM  3815  ND1 HIS B 237     18.460  92.771  56.126  1.00 14.41    B   N
ATOM  3816  CE1 HIS B 237     18.423  94.006  56.593  1.00 18.35    B   C
ATOM  3817  NE2 HIS B 237     17.413  94.638  56.023  1.00 14.90    B   N
ATOM  3818  C   HIS B 237     17.705  89.961  52.437  1.00 13.01    B   C
ATOM  3819  O   HIS B 237     16.725  89.860  51.702  1.00 12.07    B   O
ATOM  3820  N   ALA B 238     18.554  88.967  52.665  1.00 12.63    B   N
ATOM  3821  CA  ALA B 238     18.387  87.671  52.022  1.00 11.54    B   C
ATOM  3822  CB  ALA B 238     19.018  87.700  50.639  1.00  9.85    B   C
ATOM  3823  C   ALA B 238     19.010  86.554  52.836  1.00 14.48    B   C
ATOM  3824  O   ALA B 238     19.998  86.765  53.533  1.00 14.69    B   O
ATOM  3825  N   SER B 239     18.424  85.364  52.741  1.00 14.68    B   N
ATOM  3826  CA  SER B 239     18.948  84.202  53.447  1.00 14.80    B   C
ATOM  3827  CB  SER B 239     17.862  83.141  53.608  1.00 13.43    B   C
ATOM  3828  OG  SER B 239     17.340  82.758  52.355  1.00 13.26    B   O
ATOM  3829  C   SER B 239     20.104  83.656  52.614  1.00 14.91    B   C
ATOM  3830  O   SER B 239     20.945  82.902  53.107  1.00 12.99    B   O
ATOM  3831  N   GLY B 240     20.134  84.050  51.344  1.00 14.12    B   N
ATOM  3832  CA  GLY B 240     21.197  83.631  50.455  1.00 15.59    B   C
ATOM  3833  C   GLY B 240     22.217  84.752  50.346  1.00 16.66    B   C
ATOM  3834  O   GLY B 240     22.520  85.416  51.334  1.00 16.99    B   O
ATOM  3835  N   ASP B 241     22.732  84.985  49.145  1.00 15.94    B   N
ATOM  3836  CA  ASP B 241     23.722  86.036  48.947  1.00 17.18    B   C
ATOM  3837  CB  ASP B 241     24.487  85.795  47.649  1.00 18.32    B   C
ATOM  3838  CG  ASP B 241     25.703  86.673  47.527  1.00 21.73    B   C
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Figure 4PPP

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ATOM  3839 OD1 ASP B 241     25.702  87.771  48.126  1.00 22.80    B   O
ATOM  3840 OD2 ASP B 241     26.653  86.277  46.824  1.00 23.86    B   O
ATOM  3841 C   ASP B 241     23.070  87.416  48.899  1.00 15.91    B   C
ATOM  3842 O   ASP B 241     22.566  87.838  47.855  1.00 18.69    B   O
ATOM  3843 N   VAL B 242     23.091  88.125  50.022  1.00 15.82    B   N
ATOM  3844 CA  VAL B 242     22.480  89.447  50.079  1.00 15.47    B   C
ATOM  3845 CB  VAL B 242     22.373  89.961  51.538  1.00 14.55    B   C
ATOM  3846 CG1 VAL B 242     23.753  90.329  52.079  1.00 14.67    B   C
ATOM  3847 CG2 VAL B 242     21.405  91.147  51.599  1.00 13.95    B   C
ATOM  3848 C   VAL B 242     23.230  90.480  49.242  1.00 16.20    B   C
ATOM  3849 O   VAL B 242     22.624  91.396  48.693  1.00 16.97    B   O
ATOM  3850 N   ILE B 243     24.546  90.347  49.145  1.00 15.87    B   N
ATOM  3851 CA  ILE B 243     25.307  91.303  48.351  1.00 15.88    B   C
ATOM  3852 CB  ILE B 243     26.833  91.076  48.512  1.00 17.32    B   C
ATOM  3853 CG2 ILE B 243     27.606  91.924  47.510  1.00 17.19    B   C
ATOM  3854 CG1 ILE B 243     27.249  91.447  49.940  1.00 19.37    B   C
ATOM  3855 CD1 ILE B 243     28.685  91.096  50.286  1.00 19.42    B   C
ATOM  3856 C   ILE B 243     24.882  91.191  46.889  1.00 14.23    B   C
ATOM  3857 O   ILE B 243     24.745  92.200  46.201  1.00 14.19    B   O
ATOM  3858 N   TRP B 244     24.651  89.967  46.421  1.00 14.60    B   N
ATOM  3859 CA  TRP B 244     24.207  89.756  45.046  1.00 14.98    B   C
ATOM  3860 CB  TRP B 244     24.078  88.264  44.729  1.00 15.60    B   C
ATOM  3861 CG  TRP B 244     23.575  87.999  43.329  1.00 16.65    B   C
ATOM  3862 CD2 TRP B 244     22.210  87.806  42.930  1.00 19.35    B   C
ATOM  3863 CE2 TRP B 244     22.206  87.617  41.527  1.00 18.45    B   C
ATOM  3864 CE3 TRP B 244     20.989  87.775  43.622  1.00 18.90    B   C
ATOM  3865 CD1 TRP B 244     24.321  87.924  42.184  1.00 18.57    B   C
ATOM  3866 NE1 TRP B 244     23.506  87.694  41.097  1.00 17.92    B   N
ATOM  3867 CZ2 TRP B 244     21.029  87.398  40.803  1.00 17.47    B   C
ATOM  3868 CZ3 TRP B 244     19.818  87.558  42.902  1.00 18.34    B   C
ATOM  3869 CH2 TRP B 244     19.847  87.371  41.504  1.00 17.51    B   C
ATOM  3870 C   TRP B 244     22.845  90.409  44.850  1.00 16.58    B   C
ATOM  3871 O   TRP B 244     22.616  91.102  43.859  1.00 17.56    B   O
ATOM  3872 N   LEU B 245     21.937  90.180  45.796  1.00 15.30    B   N
ATOM  3873 CA  LEU B 245     20.599  90.749  45.707  1.00 15.38    B   C
ATOM  3874 CB  LEU B 245     19.746  90.306  46.900  1.00 14.42    B   C
ATOM  3875 CG  LEU B 245     18.287  90.782  46.894  1.00 12.51    B   C
ATOM  3876 CD1 LEU B 245     17.536  90.163  45.723  1.00 15.01    B   C
ATOM  3877 CD2 LEU B 245     17.618  90.397  48.215  1.00 15.46    B   C
ATOM  3878 C   LEU B 245     20.648  92.270  45.660  1.00 15.93    B   C
ATOM  3879 O   LEU B 245     19.895  92.901  44.916  1.00 11.84    B   O
ATOM  3880 N   GLU B 246     21.534  92.865  46.454  1.00 16.60    B   N
ATOM  3881 CA  GLU B 246     21.636  94.317  46.480  1.00 17.29    B   C
ATOM  3882 CB  GLU B 246     22.496  94.782  47.658  1.00 18.17    B   C
ATOM  3883 CG  GLU B 246     21.896  94.455  49.020  1.00 19.87    B   C
ATOM  3884 CD  GLU B 246     22.776  94.908  50.176  1.00 21.82    B   C
ATOM  3885 OE1 GLU B 246     24.001  94.687  50.101  1.00 23.59    B   O
ATOM  3886 OE2 GLU B 246     22.244  95.471  51.161  1.00 18.84    B   O
ATOM  3887 C   GLU B 246     22.213  94.819  45.171  1.00 19.10    B   C
ATOM  3888 O   GLU B 246     21.866  95.905  44.711  1.00 18.10    B   O
ATOM  3889 N   ARG B 247     23.082  94.016  44.564  1.00 20.90    B   N
ATOM  3890 CA  ARG B 247     23.694  94.384  43.296  1.00 21.36    B   C
ATOM  3891 CB  ARG B 247     24.819  93.407  42.945  1.00 23.57    B   C
ATOM  3892 CG  ARG B 247     25.698  93.843  41.780  1.00 28.81    B   C
ATOM  3893 CD  ARG B 247     26.796  92.813  41.516  1.00 31.64    B   C
ATOM  3894 NE  ARG B 247     27.648  92.622  42.688  1.00 33.01    B   N
ATOM  3895 CZ  ARG B 247     27.953  91.437  43.214  1.00 34.15    B   C
ATOM  3896 NH1 ARG B 247     27.475  90.319  42.678  1.00 32.31    B   N
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Figure 4QQQ

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ATOM  3897 NH2 ARG B 247     28.742  91.372  44.281  1.00 32.59    B   N
ATOM  3898  C  ARG B 247     22.612  94.369  42.218  1.00 21.28    B   C
ATOM  3899  O  ARG B 247     22.613  95.212  41.319  1.00 18.68    B   O
ATOM  3900  N  GLN B 248     21.689  93.411  42.316  1.00 19.88    B   N
ATOM  3901  CA  GLN B 248    20.587  93.310  41.359  1.00 18.33    B   C
ATOM  3902  CB  GLN B 248    19.778  92.027  41.586  1.00 16.87    B   C
ATOM  3903  CG  GLN B 248    20.458  90.749  41.119  1.00 17.30    B   C
ATOM  3904  CD  GLN B 248    20.794  90.768  39.631  1.00 21.87    B   C
ATOM  3905  OE1 GLN B 248    19.946  91.077  38.790  1.00 23.30    B   O
ATOM  3906  NE2 GLN B 248    22.032  90.423  39.304  1.00 24.03    B   N
ATOM  3907  C  GLN B 248     19.670  94.518  41.528  1.00 17.34    B   C
ATOM  3908  O  GLN B 248     19.166  95.071  40.550  1.00 16.87    B   O
ATOM  3909  N  ALA B 249     19.451  94.917  42.777  1.00 15.06    B   N
ATOM  3910  CA  ALA B 249    18.598  96.069  43.059  1.00 17.68    B   C
ATOM  3911  CB  ALA B 249    18.435  96.240  44.557  1.00 14.89    B   C
ATOM  3912  C  ALA B 249     19.210  97.332  42.449  1.00 16.19    B   C
ATOM  3913  O  ALA B 249     18.509  98.166  41.878  1.00 15.71    B   O
ATOM  3914  N  LYS B 250     20.523  97.466  42.578  1.00 15.67    B   N
ATOM  3915  CA  LYS B 250    21.221  98.625  42.039  1.00 16.75    B   C
ATOM  3916  CB  LYS B 250    22.686  98.599  42.493  1.00 20.71    B   C
ATOM  3917  CG  LYS B 250    23.555  99.725  41.952  1.00 24.70    B   C
ATOM  3918  CD  LYS B 250    23.089 101.093  42.425  1.00 29.48    B   C
ATOM  3919  CE  LYS B 250    24.028 102.180  41.914  1.00 34.06    B   C
ATOM  3920  NZ  LYS B 250    23.548 103.549  42.249  1.00 35.09    B   N
ATOM  3921  C  LYS B 250     21.137  98.633  40.514  1.00 16.02    B   C
ATOM  3922  O  LYS B 250     20.910  99.672  39.899  1.00 16.61    B   O
ATOM  3923  N  GLU B 251     21.300  97.464  39.907  1.00 16.92    B   N
ATOM  3924  CA  GLU B 251    21.256  97.366  38.457  1.00 16.87    B   C
ATOM  3925  CB  GLU B 251    21.789  96.009  38.000  1.00 17.15    B   C
ATOM  3926  CG  GLU B 251    21.913  95.902  36.492  1.00 19.76    B   C
ATOM  3927  CD  GLU B 251    22.195  94.495  36.030  1.00 21.03    B   C
ATOM  3928  OE1 GLU B 251    22.812  93.728  36.796  1.00 21.54    B   O
ATOM  3929  OE2 GLU B 251    21.813  94.159  34.891  1.00 23.50    B   O
ATOM  3930  C  GLU B 251     19.864  97.561  37.868  1.00 18.30    B   C
ATOM  3931  O  GLU B 251     19.696  98.297  36.895  1.00 18.23    B   O
ATOM  3932  N  TRP B 252     18.865  96.918  38.464  1.00 17.41    B   N
ATOM  3933  CA  TRP B 252    17.509  96.997  37.939  1.00 17.31    B   C
ATOM  3934  CB  TRP B 252    16.868  95.610  37.973  1.00 16.21    B   C
ATOM  3935  CG  TRP B 252    17.639  94.610  37.197  1.00 16.40    B   C
ATOM  3936  CD2 TRP B 252    17.650  94.459  35.775  1.00 17.43    B   C
ATOM  3937  CE2 TRP B 252    18.546  93.412  35.475  1.00 17.08    B   C
ATOM  3938  CE3 TRP B 252    16.988  95.107  34.723  1.00 20.12    B   C
ATOM  3939  CD1 TRP B 252    18.505  93.677  37.690  1.00 18.25    B   C
ATOM  3940  NE1 TRP B 252    19.053  92.954  36.662  1.00 17.57    B   N
ATOM  3941  CZ2 TRP B 252    18.799  92.996  34.167  1.00 16.27    B   C
ATOM  3942  CZ3 TRP B 252    17.239  94.691  33.416  1.00 18.36    B   C
ATOM  3943  CH2 TRP B 252    18.137  93.646  33.153  1.00 18.85    B   C
ATOM  3944  C  TRP B 252     16.555  98.000  38.565  1.00 20.68    B   C
ATOM  3945  O  TRP B 252     15.631  98.468  37.896  1.00 23.26    B   O
ATOM  3946  N  LEU B 253     16.762  98.333  39.833  1.00 20.19    B   N
ATOM  3947  CA  LEU B 253    15.878  99.279  40.508  1.00 22.15    B   C
ATOM  3948  CB  LEU B 253    15.392  98.680  41.832  1.00 19.99    B   C
ATOM  3949  CG  LEU B 253    14.796  97.269  41.748  1.00 20.08    B   C
ATOM  3950  CD1 LEU B 253    14.520  96.731  43.149  1.00 15.94    B   C
ATOM  3951  CD2 LEU B 253    13.521  97.299  40.918  1.00 20.16    B   C
ATOM  3952  C  LEU B 253     16.588 100.602  40.766  1.00 25.98    B   C
ATOM  3953  O  LEU B 253     15.971 101.573  41.213  1.00 28.88    B   O
ATOM  3954  N  LYS B 254     17.887 100.631  40.478  1.00 28.33    B   N
```

Figure 4RRR

```
ATOM  3955 CA  LYS B 254     18.713 101.822  40.684  1.00 32.00      B   C
ATOM  3956 CB  LYS B 254     18.210 102.985  39.818  1.00 33.97      B   C
ATOM  3957 CG  LYS B 254     17.844 102.597  38.388  1.00 37.77      B   C
ATOM  3958 CD  LYS B 254     18.983 101.890  37.661  1.00 38.80      B   C
ATOM  3959 CE  LYS B 254     18.544 101.453  36.265  1.00 41.63      B   C
ATOM  3960 NZ  LYS B 254     19.608 100.705  35.535  1.00 41.49      B   N
ATOM  3961 C   LYS B 254     18.677 102.214  42.162  1.00 32.29      B   C
ATOM  3962 O   LYS B 254     18.716 103.399  42.511  1.00 32.23      B   O
ATOM  3963 N   LEU B 255     18.603 101.201  43.022  1.00 31.24      B   N
ATOM  3964 CA  LEU B 255     18.560 101.397  44.469  1.00 34.52      B   C
ATOM  3965 CB  LEU B 255     17.250 100.844  45.039  1.00 34.04      B   C
ATOM  3966 CG  LEU B 255     15.917 101.437  44.584  1.00 36.59      B   C
ATOM  3967 CD1 LEU B 255     14.795 100.596  45.162  1.00 35.66      B   C
ATOM  3968 CD2 LEU B 255     15.791 102.888  45.036  1.00 36.85      B   C
ATOM  3969 C   LEU B 255     19.727 100.667  45.132  1.00 35.40      B   C
ATOM  3970 O   LEU B 255     20.326  99.794  44.473  1.00 34.56      B   O
ATOM  3971 OXT LEU B 255     20.014 100.959  46.310  1.00 38.02      B   O
ATOM  4058 OH2 TIP S   1     26.694  70.185  39.535  1.00 10.43      S   O
ATOM  4059 OH2 TIP S   2     26.903  61.775  37.433  1.00 10.86      S   O
ATOM  4060 OH2 TIP S   3     35.118  64.928  45.661  1.00  9.77      S   O
ATOM  4061 OH2 TIP S   4      3.740  88.714  42.243  1.00 12.17      S   O
ATOM  4062 OH2 TIP S   5     -3.817  87.331  48.367  1.00 15.62      S   O
ATOM  4063 OH2 TIP S   6     16.515  80.411  54.861  1.00 15.64      S   O
ATOM  4064 OH2 TIP S   7     26.620  62.820  41.255  1.00 10.32      S   O
ATOM  4065 OH2 TIP S   8      3.173  81.112  41.277  1.00 12.87      S   O
ATOM  4066 OH2 TIP S   9     -5.009  77.145  39.859  1.00 14.54      S   O
ATOM  4067 OH2 TIP S  10     17.072  78.274  43.100  1.00 15.49      S   O
ATOM  4068 OH2 TIP S  11     11.094  82.014  54.953  1.00 13.66      S   O
ATOM  4069 OH2 TIP S  12     23.114  78.487  54.347  1.00 14.98      S   O
ATOM  4070 OH2 TIP S  13     20.046  86.513  47.218  1.00 13.55      S   O
ATOM  4071 OH2 TIP S  14      2.655  89.017  38.291  1.00 15.07      S   O
ATOM  4072 OH2 TIP S  15      9.228  70.350  55.121  1.00 12.46      S   O
ATOM  4073 OH2 TIP S  16     16.739  84.862  44.381  1.00 12.76      S   O
ATOM  4074 OH2 TIP S  17     25.567  61.078  39.581  1.00 14.41      S   O
ATOM  4075 OH2 TIP S  18     37.252  56.626  40.690  1.00 14.19      S   O
ATOM  4076 OH2 TIP S  19     18.275  89.911  32.191  1.00 17.34      S   O
ATOM  4077 OH2 TIP S  20     34.008  72.385  38.024  1.00 14.04      S   O
ATOM  4078 OH2 TIP S  21     -1.688  79.172  55.257  1.00 19.38      S   O
ATOM  4079 OH2 TIP S  22     22.366  80.667  29.821  1.00 24.75      S   O
ATOM  4080 OH2 TIP S  23     12.380  75.091  59.029  1.00 20.05      S   O
ATOM  4081 OH2 TIP S  24     22.730  75.591  37.990  1.00 18.05      S   O
ATOM  4082 OH2 TIP S  25     -4.035  89.431  50.414  1.00 17.74      S   O
ATOM  4083 OH2 TIP S  26      4.573  89.940  39.949  1.00 14.11      S   O
ATOM  4084 OH2 TIP S  27     -1.906  87.737  40.180  1.00 17.43      S   O
ATOM  4085 OH2 TIP S  28     10.589  69.698  44.737  1.00 21.71      S   O
ATOM  4086 OH2 TIP S  29     25.201  95.439  52.148  1.00 16.83      S   O
ATOM  4087 OH2 TIP S  30     -8.367  85.700  23.246  1.00 15.98      S   O
ATOM  4088 OH2 TIP S  31     35.982  63.130  47.769  1.00 15.06      S   O
ATOM  4089 OH2 TIP S  32     21.296  70.481  54.804  1.00 19.30      S   O
ATOM  4090 OH2 TIP S  33     20.570  73.504  39.900  1.00 18.13      S   O
ATOM  4091 OH2 TIP S  34     27.666  49.772  40.587  1.00 14.52      S   O
ATOM  4092 OH2 TIP S  35      9.700  74.285  55.955  1.00 16.17      S   O
ATOM  4093 OH2 TIP S  36     12.186  64.800  48.529  1.00 17.60      S   O
ATOM  4094 OH2 TIP S  37     13.322  82.831  56.421  1.00 13.15      S   O
ATOM  4095 OH2 TIP S  38     34.693  38.751  49.392  1.00 20.67      S   O
ATOM  4096 OH2 TIP S  39     -5.001  91.649  54.454  1.00 20.34      S   O
ATOM  4097 OH2 TIP S  40     15.761  67.824  58.496  1.00 21.39      S   O
ATOM  4098 OH2 TIP S  41     11.148  84.424  43.877  1.00 12.67      S   O
```

Figure 4SSS

```
ATOM  4099 OH2 TIP S  42      37.642  61.003  46.856  1.00 17.93      S   O
ATOM  4100 OH2 TIP S  43      -4.373  79.173  41.785  1.00 16.71      S   O
ATOM  4101 OH2 TIP S  44      43.723  52.077  51.584  1.00 18.94      S   O
ATOM  4102 OH2 TIP S  45      20.137  97.010  51.207  1.00 22.61      S   O
ATOM  4103 OH2 TIP S  46      -4.186  94.391  33.354  1.00 24.48      S   O
ATOM  4104 OH2 TIP S  47      10.434  59.744  34.860  1.00 20.09      S   O
ATOM  4105 OH2 TIP S  48      11.296  69.306  47.243  1.00 20.43      S   O
ATOM  4106 OH2 TIP S  49      13.514  84.678  43.033  1.00 17.25      S   O
ATOM  4107 OH2 TIP S  50      27.738  70.677  61.698  1.00 22.46      S   O
ATOM  4108 OH2 TIP S  51      16.289  72.356  55.129  1.00 13.74      S   O
ATOM  4109 OH2 TIP S  52      -4.477  95.904  37.489  1.00 27.31      S   O
ATOM  4110 OH2 TIP S  53      34.164  74.207  35.803  1.00 16.19      S   O
ATOM  4111 OH2 TIP S  54      13.181  73.070  43.734  1.00 17.17      S   O
ATOM  4112 OH2 TIP S  55      -3.958  90.260  57.512  1.00 25.11      S   O
ATOM  4113 OH2 TIP S  56      30.703  42.485  54.038  1.00 21.11      S   O
ATOM  4114 OH2 TIP S  57      30.922  56.349  27.885  1.00 20.13      S   O
ATOM  4115 OH2 TIP S  58      14.662  74.601  55.720  1.00 22.72      S   O
ATOM  4116 OH2 TIP S  59      38.507  59.138  50.812  1.00 19.14      S   O
ATOM  4117 OH2 TIP S  60      42.816  67.475  28.609  1.00 20.79      S   O
ATOM  4118 OH2 TIP S  61      -6.400  95.465  43.206  1.00 18.25      S   O
ATOM  4119 OH2 TIP S  62       6.561 102.864  47.606  1.00 21.89      S   O
ATOM  4120 OH2 TIP S  63      35.560  76.427  29.271  1.00 20.86      S   O
ATOM  4121 OH2 TIP S  64       5.810  69.019  32.123  1.00 25.31      S   O
ATOM  4122 OH2 TIP S  65      30.127  54.457  33.804  1.00 22.20      S   O
ATOM  4123 OH2 TIP S  66      14.517  98.509  59.915  1.00 20.97      S   O
ATOM  4124 OH2 TIP S  67      20.921  81.728  55.488  1.00 15.12      S   O
ATOM  4125 OH2 TIP S  68      18.125  78.127  55.061  1.00 22.38      S   O
ATOM  4126 OH2 TIP S  69       4.578 106.224  53.414  1.00 23.88      S   O
ATOM  4127 OH2 TIP S  70     -13.259  95.151  42.403  1.00 22.02      S   O
ATOM  4128 OH2 TIP S  71      19.506  66.848  43.948  1.00 14.64      S   O
ATOM  4129 OH2 TIP S  72      20.492  58.168  29.357  1.00 24.23      S   O
ATOM  4130 OH2 TIP S  73      14.362  66.682  45.311  1.00 21.95      S   O
ATOM  4131 OH2 TIP S  74      37.948  64.500  49.199  1.00 22.89      S   O
ATOM  4132 OH2 TIP S  75      22.382  83.107  46.881  1.00 21.36      S   O
ATOM  4133 OH2 TIP S  76       2.257  71.707  33.743  1.00 22.26      S   O
ATOM  4134 OH2 TIP S  77      28.562  50.607  60.811  1.00 23.59      S   O
ATOM  4135 OH2 TIP S  78      12.908  55.269  54.605  1.00 22.04      S   O
ATOM  4136 OH2 TIP S  79      23.712  82.581  52.850  1.00 18.46      S   O
ATOM  4137 OH2 TIP S  80       6.000  64.702  50.376  1.00 22.24      S   O
ATOM  4138 OH2 TIP S  81      31.597  63.665  38.013  1.00 16.06      S   O
ATOM  4139 OH2 TIP S  82       3.204 101.393  39.851  1.00 18.09      S   O
ATOM  4140 OH2 TIP S  83      -3.695  88.746  62.013  1.00 24.84      S   O
ATOM  4141 OH2 TIP S  84      17.546  65.110  21.326  1.00 19.55      S   O
ATOM  4142 OH2 TIP S  85      26.824  59.347  62.759  1.00 26.30      S   O
ATOM  4143 OH2 TIP S  86      29.013  78.700  36.194  1.00 29.19      S   O
ATOM  4144 OH2 TIP S  87     -21.912  84.760  37.477  1.00 26.29      S   O
ATOM  4145 OH2 TIP S  88      37.659  49.564  54.905  1.00 21.54      S   O
ATOM  4146 OH2 TIP S  89      15.623  89.654  61.494  1.00 20.60      S   O
ATOM  4147 OH2 TIP S  90      46.913  73.636  27.864  1.00 24.09      S   O
ATOM  4148 OH2 TIP S  91      31.635  68.716  13.795  1.00 26.68      S   O
ATOM  4149 OH2 TIP S  92       8.998  77.444  41.106  1.00 21.52      S   O
ATOM  4150 OH2 TIP S  93      19.563  69.848  56.803  1.00 23.78      S   O
ATOM  4151 OH2 TIP S  94      21.054  77.796  57.903  1.00 20.91      S   O
ATOM  4152 OH2 TIP S  95      39.029  70.195  42.752  1.00 19.43      S   O
ATOM  4153 OH2 TIP S  96      16.357  59.879  28.472  1.00 34.72      S   O
ATOM  4154 OH2 TIP S  97       6.277  85.600  21.656  1.00 18.30      S   O
ATOM  4155 OH2 TIP S  98      24.381  79.010  25.797  1.00 24.45      S   O
ATOM  4156 OH2 TIP S  99      -0.330  73.515  46.326  1.00 21.44      S   O
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Figure 4TTT

```
ATOM  4157  OH2 TIP S 100     19.996  63.469  21.479  1.00 20.07      S   O
ATOM  4158  OH2 TIP S 101      8.484  64.804  37.057  1.00 21.03      S   O
ATOM  4159  OH2 TIP S 102     18.063  76.067  36.689  1.00 20.99      S   O
ATOM  4160  OH2 TIP S 103     13.804  68.104  43.044  1.00 25.16      S   O
ATOM  4161  OH2 TIP S 104     10.019  70.355  50.629  1.00 23.39      S   O
ATOM  4162  OH2 TIP S 105     36.764  63.450  55.390  1.00 19.23      S   O
ATOM  4163  OH2 TIP S 106     -3.017  81.106  52.043  1.00 29.08      S   O
ATOM  4164  OH2 TIP S 107     33.894  73.874  51.602  1.00 22.56      S   O
ATOM  4165  OH2 TIP S 108    -10.562  79.620  30.884  1.00 25.06      S   O
ATOM  4166  OH2 TIP S 109     -3.241  87.887  16.187  1.00 22.20      S   O
ATOM  4167  OH2 TIP S 110     36.320  79.997  40.961  1.00 30.47      S   O
ATOM  4168  OH2 TIP S 111     12.536  71.003  57.233  1.00 20.62      S   O
ATOM  4169  OH2 TIP S 112     -0.943  95.950  34.554  1.00 25.68      S   O
ATOM  4170  OH2 TIP S 113     14.938  45.779  46.539  1.00 32.69      S   O
ATOM  4171  OH2 TIP S 114     44.541  72.750  24.779  1.00 28.57      S   O
ATOM  4172  OH2 TIP S 115     16.028  56.338  61.884  1.00 27.69      S   O
ATOM  4173  OH2 TIP S 116     25.959  84.862  44.510  1.00 22.27      S   O
ATOM  4174  OH2 TIP S 117     11.898  70.641  40.303  1.00 29.38      S   O
ATOM  4175  OH2 TIP S 118     20.005  82.352  45.778  1.00 23.69      S   O
ATOM  4176  OH2 TIP S 119     24.653  82.113  42.509  1.00 26.73      S   O
ATOM  4177  OH2 TIP S 120     39.045  70.244  55.129  1.00 26.86      S   O
ATOM  4178  OH2 TIP S 121    -14.861  94.263  30.815  1.00 25.70      S   O
ATOM  4179  OH2 TIP S 122     28.805  79.348  55.384  1.00 24.42      S   O
ATOM  4180  OH2 TIP S 123     34.409  78.819  35.704  1.00 22.51      S   O
ATOM  4181  OH2 TIP S 124     25.708  95.887  48.431  1.00 22.52      S   O
ATOM  4182  OH2 TIP S 125     20.200  81.715  43.235  1.00 28.28      S   O
ATOM  4183  OH2 TIP S 126      8.358  89.545  27.306  1.00 25.44      S   O
ATOM  4184  OH2 TIP S 127     28.451  42.142  55.370  1.00 32.71      S   O
ATOM  4185  OH2 TIP S 128     -1.140  72.535  35.377  1.00 25.03      S   O
ATOM  4186  OH2 TIP S 129     42.723  73.261  29.197  1.00 26.01      S   O
ATOM  4187  OH2 TIP S 130      0.475 106.754  43.565  1.00 35.60      S   O
ATOM  4188  OH2 TIP S 131     -8.799  81.517  47.238  1.00 30.82      S   O
ATOM  4189  OH2 TIP S 132     18.817  63.647  62.682  1.00 23.39      S   O
ATOM  4190  OH2 TIP S 133    -14.788  83.367  33.703  1.00 22.25      S   O
ATOM  4191  OH2 TIP S 134     28.486  47.289  40.587  1.00 26.04      S   O
ATOM  4192  OH2 TIP S 135     13.709  66.288  58.292  1.00 31.84      S   O
ATOM  4193  OH2 TIP S 136      4.869  72.011  43.934  1.00 21.85      S   O
ATOM  4194  OH2 TIP S 137    -19.103  77.442  35.205  1.00 29.80      S   O
ATOM  4195  OH2 TIP S 138     20.407  79.490  35.831  1.00 35.16      S   O
ATOM  4196  OH2 TIP S 139     10.860  84.010  22.443  1.00 27.02      S   O
ATOM  4197  OH2 TIP S 140      0.151 101.506  60.922  1.00 25.88      S   O
ATOM  4198  OH2 TIP S 141     31.584  47.279  41.254  1.00 23.80      S   O
ATOM  4199  OH2 TIP S 142     38.066  70.701  25.990  1.00 19.24      S   O
ATOM  4200  OH2 TIP S 143     44.977  72.631  31.204  1.00 23.78      S   O
ATOM  4201  OH2 TIP S 144     10.719  65.231  40.054  1.00 26.38      S   O
ATOM  4202  OH2 TIP S 145      7.475  91.297  29.034  1.00 27.02      S   O
ATOM  4203  OH2 TIP S 146     37.874  61.748  52.268  1.00 29.73      S   O
ATOM  4204  OH2 TIP S 147     -5.574  93.894  53.509  1.00 23.66      S   O
ATOM  4205  OH2 TIP S 148     17.820  78.905  36.654  1.00 28.79      S   O
ATOM  4206  OH2 TIP S 149     29.549  83.050  48.881  1.00 26.52      S   O
ATOM  4207  OH2 TIP S 150    -10.366 100.932  54.067  1.00 20.68      S   O
ATOM  4208  OH2 TIP S 151     30.504  64.646  60.794  1.00 28.37      S   O
ATOM  4209  OH2 TIP S 152     49.012  70.756  24.772  1.00 31.55      S   O
ATOM  4210  OH2 TIP S 153     30.846  45.257  57.188  1.00 31.72      S   O
ATOM  4211  OH2 TIP S 154     43.180  59.055  25.923  1.00 26.29      S   O
ATOM  4212  OH2 TIP S 155     22.523  66.585  65.647  1.00 32.96      S   O
ATOM  4213  OH2 TIP S 156      2.253 106.632  56.997  1.00 37.06      S   O
ATOM  4214  OH2 TIP S 157     21.987  90.927  36.214  1.00 24.25      S   O
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Figure 4UUU

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ATOM  4215  OH2 TIP S 158      24.995  45.779  50.248  1.00 28.19      S   O
ATOM  4216  OH2 TIP S 159      24.701  87.274  52.417  1.00 25.41      S   O
ATOM  4217  OH2 TIP S 160      19.481  54.793  61.669  1.00 24.28      S   O
ATOM  4218  OH2 TIP S 161       5.052  66.267  52.559  1.00 20.50      S   O
ATOM  4219  OH2 TIP S 162      24.083  47.425  48.238  1.00 32.20      S   O
ATOM  4220  OH2 TIP S 163      50.567  67.161  31.028  1.00 21.83      S   O
ATOM  4221  OH2 TIP S 164      15.358  64.805  23.213  1.00 24.49      S   O
ATOM  4222  OH2 TIP S 165      -1.913  91.256  42.961  1.00 21.23      S   O
ATOM  4223  OH2 TIP S 166      32.576  60.552  40.991  1.00 24.61      S   O
ATOM  4224  OH2 TIP S 167       5.829  70.768  57.525  1.00 22.41      S   O
ATOM  4225  OH2 TIP S 168       6.357  83.074  62.946  1.00 20.77      S   O
ATOM  4226  OH2 TIP S 169      28.962  85.053  47.200  1.00 36.42      S   O
ATOM  4227  OH2 TIP S 170      22.828  55.785  37.965  1.00 34.04      S   O
ATOM  4228  OH2 TIP S 171       9.903 109.166  51.388  1.00 29.79      S   O
ATOM  4229  OH2 TIP S 172       6.629  71.093  33.592  1.00 24.39      S   O
ATOM  4230  OH2 TIP S 173      24.428  80.747  55.009  1.00 17.22      S   O
ATOM  4231  OH2 TIP S 174      11.049  67.896  25.243  1.00 28.73      S   O
ATOM  4232  OH2 TIP S 175      26.525  84.672  50.346  1.00 22.59      S   O
ATOM  4233  OH2 TIP S 176      14.485  79.387  59.276  1.00 36.33      S   O
ATOM  4234  OH2 TIP S 178      -8.133  88.350  22.930  1.00 24.98      S   O
ATOM  4235  OH2 TIP S 179      11.008  89.282  26.933  1.00 26.38      S   O
ATOM  4236  OH2 TIP S 180      29.198  77.232  57.047  1.00 28.34      S   O
ATOM  4237  OH2 TIP S 181      42.985  63.495  21.723  1.00 32.93      S   O
ATOM  4238  OH2 TIP S 182      -2.488  92.239  26.844  1.00 31.41      S   O
ATOM  4239  OH2 TIP S 183      38.070  68.391  49.950  1.00 27.44      S   O
ATOM  4240  OH2 TIP S 184       3.026  87.382  17.697  1.00 24.17      S   O
ATOM  4241  OH2 TIP S 185      32.032  45.265  50.288  1.00 26.40      S   O
ATOM  4242  OH2 TIP S 186      39.904  55.447  42.177  1.00 25.49      S   O
ATOM  4243  OH2 TIP S 187       2.867  70.555  28.600  1.00 25.55      S   O
ATOM  4244  OH2 TIP S 188      28.784  77.898  31.205  1.00 27.78      S   O
ATOM  4245  OH2 TIP S 189       6.525  74.751  39.761  1.00 27.53      S   O
ATOM  4246  OH2 TIP S 190      -6.708  81.142  14.878  1.00 30.15      S   O
ATOM  4247  OH2 TIP S 191      23.949  87.249  38.410  1.00 26.94      S   O
ATOM  4248  OH2 TIP S 192       5.279  83.214  19.647  1.00 23.04      S   O
ATOM  4249  OH2 TIP S 193       7.787  93.915  65.832  1.00 34.56      S   O
ATOM  4250  OH2 TIP S 194      40.056  62.665  49.571  1.00 45.56      S   O
ATOM  4251  OH2 TIP S 195      17.005  83.158  42.309  1.00 26.09      S   O
ATOM  4252  OH2 TIP S 196      39.783  52.482  36.066  1.00 43.89      S   O
ATOM  4253  OH2 TIP S 197      21.034  85.408  34.631  1.00 21.18      S   O
ATOM  4254  OH2 TIP S 198      -2.760  93.994  35.518  1.00 32.71      S   O
ATOM  4255  OH2 TIP S 199     -14.876  77.201  34.781  1.00 29.91      S   O
ATOM  4256  OH2 TIP S 200       7.796  94.208  62.630  1.00 34.21      S   O
ATOM  4257  OH2 TIP S 201     -10.407  94.563  54.451  1.00 30.66      S   O
ATOM  4258  OH2 TIP S 202      19.132  85.088  38.251  1.00 26.36      S   O
ATOM  4259  OH2 TIP S 203      46.329  71.427  42.245  1.00 38.45      S   O
ATOM  4260  OH2 TIP S 204      38.151  49.728  42.054  1.00 23.90      S   O
ATOM  4261  OH2 TIP S 205     -16.881  92.357  37.722  1.00 29.19      S   O
ATOM  4262  OH2 TIP S 206       8.018  58.831  39.198  1.00 17.50      S   O
ATOM  4263  OH2 TIP S 207      23.689  77.990  32.612  1.00 37.51      S   O
ATOM  4264  OH2 TIP S 208      30.303  45.065  54.676  1.00 28.16      S   O
ATOM  4265  OH2 TIP S 209      25.161  84.823  52.568  1.00 29.69      S   O
ATOM  4266  OH2 TIP S 210      23.062  78.703  21.684  1.00 26.51      S   O
ATOM  4267  OH2 TIP S 211      26.355  47.512  59.226  1.00 41.38      S   O
ATOM  4268  OH2 TIP S 212      12.364  73.834  56.670  1.00 17.58      S   O
ATOM  4269  OH2 TIP S 213      22.789 101.251  38.634  1.00 36.48      S   O
ATOM  4270  OH2 TIP S 214      30.444  78.274  42.812  1.00 18.27      S   O
ATOM  4271  OH2 TIP S 215      16.714  66.636  43.404  1.00 27.82      S   O
ATOM  4272  OH2 TIP S 216      11.118 110.647  48.883  1.00 41.21      S   O
```

Figure 4VVV

```
ATOM  4273  OH2 TIP S 217     11.938  77.223  62.477  1.00 26.78      S   O
ATOM  4274  OH2 TIP S 218     21.348  98.318  46.299  1.00 22.54      S   O
ATOM  4275  OH2 TIP S 219      6.335  90.109  61.055  1.00 30.93      S   O
ATOM  4276  OH2 TIP S 220     16.849  58.092  31.635  1.00 27.78      S   O
ATOM  4277  OH2 TIP S 221    -14.977  98.435  36.110  1.00 29.94      S   O
ATOM  4278  OH2 TIP S 222     32.209  56.644  34.417  1.00 27.61      S   O
ATOM  4279  OH2 TIP S 223     38.616  69.338  19.683  1.00 35.00      S   O
ATOM  4280  OH2 TIP S 224     43.793  66.187  40.980  1.00 28.57      S   O
ATOM  4281  OH2 TIP S 225     25.865  49.291  48.912  1.00 22.19      S   O
ATOM  4282  OH2 TIP S 226     29.493  51.282  39.294  1.00 28.59      S   O
ATOM  4283  OH2 TIP S 227      8.557  68.734  23.715  1.00 32.38      S   O
ATOM  4284  OH2 TIP S 228     35.030  72.215  49.061  1.00 21.47      S   O
ATOM  4285  OH2 TIP S 229     -5.863  84.407  53.693  1.00 32.71      S   O
ATOM  4286  OH2 TIP S 230      8.409  66.822  21.454  1.00 32.17      S   O
ATOM  4287  OH2 TIP S 231     16.090  88.535  25.766  1.00 45.41      S   O
ATOM  4288  OH2 TIP S 232      5.228  66.001  48.372  1.00 33.03      S   O
ATOM  4289  OH2 TIP S 233     22.372  81.334  39.929  1.00 38.56      S   O
ATOM  4290  OH2 TIP S 234    -11.344  82.468  23.312  1.00 32.37      S   O
ATOM  4291  OH2 TIP S 235     -5.663  88.297  52.367  1.00 28.46      S   O
ATOM  4292  OH2 TIP S 236     13.616  74.457  18.786  1.00 42.18      S   O
ATOM  4293  OH2 TIP S 237     25.283  53.133  37.923  1.00 40.56      S   O
ATOM  4294  OH2 TIP S 238      8.026  53.624  54.137  1.00 31.65      S   O
ATOM  4295  OH2 TIP S 239     34.534  62.367  11.800  1.00 31.60      S   O
ATOM  4296  OH2 TIP S 240      1.831  56.099  44.184  1.00 34.48      S   O
ATOM  4297  OH2 TIP S 241     49.497  62.599  26.810  1.00 26.78      S   O
ATOM  4298  OH2 TIP S 242     -4.758  72.368  21.533  1.00 38.11      S   O
ATOM  4299  OH2 TIP S 243     -5.868  83.431  58.623  1.00 34.40      S   O
ATOM  4300  OH2 TIP S 244     29.156  81.797  37.170  1.00 39.60      S   O
ATOM  4301  OH2 TIP S 245     21.609  85.611  37.638  1.00 20.34      S   O
ATOM  4302  OH2 TIP S 246     -4.284  77.490  49.709  1.00 35.30      S   O
ATOM  4303  OH2 TIP S 247     31.807  48.664  61.432  1.00 43.66      S   O
ATOM  4304  OH2 TIP S 248     34.652  80.273  32.759  1.00 35.30      S   O
ATOM  4305  OH2 TIP S 249     -7.767  74.088  33.904  1.00 27.76      S   O
ATOM  4306  OH2 TIP S 250     -0.973  76.943  21.093  1.00 36.81      S   O
ATOM  4307  OH2 TIP S 251     17.520 103.841  50.759  1.00 37.13      S   O
ATOM  4308  OH2 TIP S 252     36.677  59.162  23.943  1.00 39.63      S   O
ATOM  4309  OH2 TIP S 253     -3.985  93.307  65.493  1.00 38.58      S   O
ATOM  4310  OH2 TIP S 254     26.053  53.836  34.851  1.00 37.31      S   O
ATOM  4311  OH2 TIP S 255     -7.010  78.156  28.377  1.00 28.40      S   O
ATOM  4312  OH2 TIP S 256      3.198  69.864  24.836  1.00 24.87      S   O
ATOM  4313  OH2 TIP S 257     -2.729  89.793  59.984  1.00 35.90      S   O
ATOM  4314  OH2 TIP S 259     12.874  62.780  21.486  1.00 40.71      S   O
ATOM  4315  OH2 TIP S 260     34.460  53.900  62.259  1.00 37.85      S   O
ATOM  4316  OH2 TIP S 261      8.524  50.114  40.677  1.00 29.93      S   O
ATOM  4317  OH2 TIP S 262     13.534  51.901  52.802  1.00 35.55      S   O
ATOM  4318  OH2 TIP S 263     -5.651  71.332  27.984  1.00 36.22      S   O
ATOM  4319  OH2 TIP S 264     10.884  74.117  37.648  1.00 23.87      S   O
ATOM  4320  OH2 TIP S 265      1.558 105.085  59.290  1.00 30.99      S   O
ATOM  4321  OH2 TIP S 267     22.855  87.241  54.244  1.00 39.85      S   O
ATOM  4322  OH2 TIP S 268     19.606  84.810  44.816  1.00 16.00      S   O
ATOM  4323  OH2 TIP S 269     10.246  57.810  32.854  1.00 25.86      S   O
ATOM  4324  OH2 TIP S 270    -21.599  79.618  39.328  1.00 38.76      S   O
ATOM  4325  OH2 TIP S 271     35.642  69.502  46.091  1.00 25.61      S   O
ATOM  4326  OH2 TIP S 272      7.124  71.606  39.935  1.00 32.52      S   O
ATOM  4327  OH2 TIP S 274     37.219  53.704  29.589  1.00 30.49      S   O
ATOM  4328  OH2 TIP S 275     15.688  71.656  41.660  1.00 35.47      S   O
ATOM  4329  OH2 TIP S 276     18.771  98.089  33.479  1.00 36.76      S   O
ATOM  4330  OH2 TIP S 277     18.891  96.723  59.037  1.00 34.81      S   O
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Figure 4WWW

```
ATOM  4331  OH2 TIP S 279      20.582  96.155  32.990  1.00 36.72      S   O
ATOM  4332  OH2 TIP S 280      38.382  46.507  54.083  1.00 22.09      S   O
ATOM  4333  OH2 TIP S 284      33.499  78.469  29.422  1.00 42.54      S   O
ATOM  4334  OH2 TIP S 285      43.663  56.107  27.511  1.00 34.42      S   O
ATOM  4335  OH2 TIP S 286      35.122  60.670  20.712  1.00 39.38      S   O
ATOM  4336  OH2 TIP S 287      -1.725  96.233  63.363  1.00 35.97      S   O
ATOM  4337  OH2 TIP S 290      18.717  83.949  40.601  1.00 23.89      S   O
ATOM  4338  OH2 TIP S 291      38.772  45.987  46.680  1.00 36.15      S   O
ATOM  4339  OH2 TIP S 292      20.224  69.382  59.695  1.00 29.64      S   O
ATOM  4340  OH2 TIP S 293       8.282  78.199  63.669  1.00 36.59      S   O
ATOM  4341  OH2 TIP S 294      14.047  63.860  59.319  1.00 44.69      S   O
ATOM  4342  OH2 TIP S 297      -5.817  72.739  40.818  1.00 38.14      S   O
ATOM  4343  OH2 TIP S 298      26.321  64.439  12.786  1.00 45.15      S   O
ATOM  4344  OH2 TIP S 299      -6.944 102.099  43.661  1.00 28.91      S   O
ATOM  4345  OH2 TIP S 300      31.982  51.444  38.891  1.00 26.30      S   O
ATOM  4346  OH2 TIP S 301      22.179  61.349  17.217  1.00 28.54      S   O
ATOM  4347  OH2 TIP S 302      11.846  66.672  46.440  1.00 15.33      S   O
ATOM  4348  OH2 TIP S 303      16.579  61.209  61.822  1.00 25.84      S   O
ATOM  4349  OH2 TIP S 304       9.179  61.102  31.089  1.00 35.18      S   O
ATOM  4350  OH2 TIP S 306      43.337  56.983  38.631  1.00 31.17      S   O
ATOM  4351  OH2 TIP S 307      -4.729  79.060  14.954  1.00 29.45      S   O
ATOM  4352  OH2 TIP S 309       3.264  96.531  34.343  1.00 35.87      S   O
ATOM  4353  OH2 TIP S 310      33.597  56.115  32.020  1.00 38.28      S   O
ATOM  4354  OH2 TIP S 312      21.131  84.199  42.642  1.00 16.36      S   O
ATOM  4355  OH2 TIP S 314      13.289  90.298  22.035  1.00 37.86      S   O
ATOM  4356  OH2 TIP S 315     -21.318  88.597  32.650  1.00 31.68      S   O
ATOM  4357  OH2 TIP S 316       0.324  97.812  61.903  1.00 28.65      S   O
ATOM  4358  OH2 TIP S 317      15.681  48.773  53.561  1.00 32.11      S   O
ATOM  4359  OH2 TIP S 318       6.414  66.203  28.644  1.00 45.39      S   O
ATOM  4360  OH2 TIP S 320      21.877  45.789  57.051  1.00 37.88      S   O
ATOM  4361  OH2 TIP S 325      33.257  76.751  48.828  1.00 36.69      S   O
ATOM  4362  OH2 TIP S 326      -1.477  99.714  39.504  1.00 31.96      S   O
ATOM  4363  OH2 TIP S 327       7.083 107.442  40.232  1.00 34.50      S   O
ATOM  4364  OH2 TIP S 328      19.455  81.284  39.450  1.00 31.13      S   O
ATOM  4365  OH2 TIP S 330      18.928  59.678  27.698  1.00 23.64      S   O
ATOM  4366  OH2 TIP S 333       2.949  68.265  43.594  1.00 46.66      S   O
ATOM  4367  OH2 TIP S 334      -8.138 104.339  45.239  1.00 36.83      S   O
ATOM  4368  OH2 TIP S 336       3.891  58.458  48.159  1.00 40.09      S   O
ATOM  4369  OH2 TIP S 339     -11.491  79.098  22.692  1.00 31.58      S   O
ATOM  4370  OH2 TIP S 342      -3.605  77.350  56.479  1.00 33.40      S   O
ATOM  4371  OH2 TIP S 345      48.945  64.149  23.906  1.00 33.98      S   O
ATOM  4372  OH2 TIP S 348      17.597  50.879  59.000  1.00 46.70      S   O
ATOM  4373  OH2 TIP S 349     -19.548  99.216  33.850  1.00 31.30      S   O
ATOM  4374  OH2 TIP S 350      11.566  66.969  42.047  1.00 25.33      S   O
ATOM  4375  OH2 TIP S 353      24.674  43.379  42.738  1.00 46.49      S   O
ATOM  4376  OH2 TIP S 354      20.654  78.836  55.418  1.00 19.53      S   O
ATOM  4377  OH2 TIP S 357      17.254  91.782  60.031  1.00 23.92      S   O
ATOM  4378  OH2 TIP S 358       9.923  67.047  44.491  1.00 20.59      S   O
ATOM  4379  OH2 TIP S 359      36.952  66.998  45.661  1.00 21.28      S   O
ATOM  4380  OH2 TIP S 360      15.012  70.447  58.501  1.00 20.49      S   O
ATOM  4381  OH2 TIP S 361      38.560  66.828  47.799  1.00 18.16      S   O
ATOM  4382  OH2 TIP S 362      12.567  70.351  43.331  1.00 21.60      S   O
ATOM  4383  OH2 TIP S 363      10.275  70.909  59.173  1.00 20.25      S   O
ATOM  4384  OH2 TIP S 365      -8.636  80.604  29.420  1.00 20.84      S   O
ATOM  4385  OH2 TIP S 366      27.535  82.312  43.508  1.00 25.30      S   O
ATOM  4386  OH2 TIP S 367      17.257  86.397  26.338  1.00 29.08      S   O
ATOM  4387  OH2 TIP S 368       4.358  55.280  44.796  1.00 40.14      S   O
ATOM  4388  OH2 TIP S 369       8.463  83.561  21.334  1.00 22.41      S   O
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Figure 4XXX

```
ATOM  4389  OH2 TIP S 370     -8.086  97.612  37.816  1.00 25.46      S   O
ATOM  4390  OH2 TIP S 371     12.843  74.928  39.116  1.00 31.70      S   O
ATOM  4391  OH2 TIP S 372      8.347  72.232  57.105  1.00 25.70      S   O
ATOM  4392  OH2 TIP S 373     -3.834 109.911  52.412  1.00 25.46      S   O
ATOM  4393  OH2 TIP S 374     38.734  67.042  43.751  1.00 25.21      S   O
ATOM  4394  OH2 TIP S 375     20.952  90.132  33.041  1.00 26.25      S   O
ATOM  4395  OH2 TIP S 376     21.122  98.404  49.083  1.00 21.33      S   O
ATOM  4396  OH2 TIP S 377    -12.795  97.771  42.948  1.00 27.19      S   O
ATOM  4397  OH2 TIP S 378     24.316  79.549  28.534  1.00 25.40      S   O
ATOM  4398  OH2 TIP S 379     27.736  88.375  45.434  1.00 29.24      S   O
ATOM  4399  OH2 TIP S 380      8.225  59.683  36.172  1.00 24.77      S   O
ATOM  4400  OH2 TIP S 381     37.450  53.227  35.003  1.00 32.48      S   O
ATOM  4401  OH2 TIP S 382    -10.586  84.900  22.199  1.00 30.47      S   O
ATOM  4402  OH2 TIP S 383    -15.137  95.854  40.707  1.00 25.76      S   O
ATOM  4403  OH2 TIP S 384     16.777  65.477  62.229  1.00 26.46      S   O
ATOM  4404  OH2 TIP S 385     28.839  86.168  50.617  1.00 33.26      S   O
ATOM  4405  OH2 TIP S 386     17.382  84.892  57.199  1.00 22.87      S   O
ATOM  4406  OH2 TIP S 387     27.000  52.190  62.926  1.00 27.15      S   O
ATOM  4407  OH2 TIP S 388     31.661  79.835  35.615  1.00 28.03      S   O
ATOM  4408  OH2 TIP S 389     -4.676  84.758  48.894  1.00 31.68      S   O
ATOM  4409  OH2 TIP S 390     -5.662  91.557  50.040  1.00 31.19      S   O
ATOM  4410  OH2 TIP S 391     23.487  83.965  44.473  1.00 28.65      S   O
ATOM  4411  OH2 TIP S 392     -6.441  88.875  58.175  1.00 33.33      S   O
ATOM  4412  OH2 TIP S 393      7.603  93.526  36.250  1.00 30.57      S   O
ATOM  4413  OH2 TIP S 394     49.203  72.825  26.301  1.00 24.46      S   O
ATOM  4414  OH2 TIP S 395     28.479  61.371  62.617  1.00 32.12      S   O
ATOM  4415  OH2 TIP S 397     -9.168  83.076  17.253  1.00 25.74      S   O
ATOM  4416  OH2 TIP S 398     16.075  88.965  63.990  1.00 30.49      S   O
ATOM  4417  OH2 TIP S 400     13.310  95.842  67.259  1.00 29.76      S   O
ATOM  4418  OH2 TIP S 401      5.918  66.938  33.592  1.00 31.14      S   O
ATOM  4419  OH2 TIP S 402      0.155 106.248  55.777  1.00 32.60      S   O
ATOM  4420  OH2 TIP S 403      6.110  92.248  62.655  1.00 27.95      S   O
ATOM  4421  OH2 TIP S 404      2.233 103.880  39.763  1.00 31.52      S   O
ATOM  4422  OH2 TIP S 405     25.694  98.715  48.972  1.00 29.93      S   O
ATOM  4423  OH2 TIP S 406     10.674  73.231  60.407  1.00 31.34      S   O
ATOM  4424  OH2 TIP S 409     51.882  66.157  29.120  1.00 26.96      S   O
ATOM  4425  OH2 TIP S 410      6.325  68.647  46.053  1.00 34.29      S   O
ATOM  4426  OH2 TIP S 412     39.391  64.285  54.825  1.00 28.64      S   O
ATOM  4427  OH2 TIP S 413     -2.620  73.079  47.858  1.00 31.55      S   O
ATOM  4428  OH2 TIP S 414     32.879  78.973  43.464  1.00 29.58      S   O
ATOM  4429  OH2 TIP S 415    -15.016  96.572  33.202  1.00 45.53      S   O
ATOM  4430  OH2 TIP S 416     39.377  75.743  32.551  1.00 30.17      S   O
ATOM  4431  OH2 TIP S 417     31.294  47.074  59.585  1.00 32.29      S   O
ATOM  4432  OH2 TIP S 418     20.908  99.085  60.072  1.00 33.84      S   O
ATOM  4433  OH2 TIP S 421     16.227  75.089  58.255  1.00 34.63      S   O
ATOM  4434  OH2 TIP S 423      9.515  68.766  41.162  1.00 31.09      S   O
ATOM  4435  OH2 TIP S 424     24.057  90.877  41.184  1.00 32.57      S   O
ATOM  4436  OH2 TIP S 425    -23.421  85.321  34.874  1.00 40.73      S   O
ATOM  4437  OH2 TIP S 426     -6.600  85.509  60.637  1.00 36.33      S   O
ATOM  4438  OH2 TIP S 429     18.068  74.274  39.152  1.00 28.30      S   O
ATOM  4439  OH2 TIP S 430      0.216  72.088  29.280  1.00 34.77      S   O
ATOM  4440  OH2 TIP S 431     24.237  97.970  52.510  1.00 40.38      S   O
ATOM  4441  OH2 TIP S 433     16.496  61.776  20.380  1.00 31.74      S   O
ATOM  4442  OH2 TIP S 434     23.656  81.140  23.402  1.00 39.14      S   O
ATOM  4443  OH2 TIP S 435     45.512  70.376  23.767  1.00 38.06      S   O
ATOM  4444  OH2 TIP S 436      5.133  69.622  42.446  1.00 33.04      S   O
ATOM  4445  OH2 TIP S 440     23.692  79.457  34.661  1.00 40.65      S   O
ATOM  4446  OH2 TIP S 443     15.889  73.328  39.832  1.00 29.37      S   O
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Figure 4YYY

```
ATOM  4447  OH2 TIP S 444     -8.745  70.532  28.410  1.00 33.62      S   O
ATOM  4448  OH2 TIP S 446     32.260  78.506  13.999  1.00 45.13      S   O
ATOM  4449  OH2 TIP S 448     39.242  48.079  43.803  1.00 33.38      S   O
ATOM  4450  OH2 TIP S 449     34.559  75.768  22.405  1.00 31.84      S   O
ATOM  4451  OH2 TIP S 450     17.344  71.627  57.656  1.00 30.16      S   O
ATOM  4452  OH2 TIP S 453     17.850  55.704  64.074  1.00 41.95      S   O
ATOM  4453  OH2 TIP S 454     12.673  87.630  65.105  1.00 36.77      S   O
ATOM  4454  OH2 TIP S 455     18.393  73.689  58.998  1.00 35.69      S   O
ATOM  4455  OH2 TIP S 457     31.350  80.284  54.849  1.00 32.98      S   O
ATOM  4456  OH2 TIP S 459     31.948  64.117  63.134  1.00 33.16      S   O
ATOM  4457  OH2 TIP S 461     25.883  44.584  58.922  1.00 26.81      S   O
ATOM  4458  OH2 TIP S 462     15.411  75.744  38.970  1.00 38.18      S   O
ATOM  4459  OH2 TIP S 465     -6.694  85.996  51.462  1.00 39.03      S   O
ATOM  4460  OH2 TIP S 467     22.428  74.991  56.119  1.00 48.69      S   O
ATOM  4461  OH2 TIP S 472      7.409  68.343  43.765  1.00 40.63      S   O
ATOM  4462  OH2 TIP S 477      3.696  81.760  15.765  1.00 41.18      S   O
ATOM  4463  OH2 TIP S 478     36.353  75.696  51.865  1.00 40.40      S   O
ATOM  4464  OH2 TIP S 479     45.063  73.009  39.613  1.00 30.28      S   O
ATOM  4465  OH2 TIP S 480     35.167  68.155  64.949  1.00 36.43      S   O
ATOM  4466  OH2 TIP S 481     16.895  81.810  19.179  1.00 26.87      S   O
ATOM  4467  OH2 TIP S 482      9.338  64.581  19.670  1.00 47.45      S   O
ATOM  4468  OH2 TIP S 486     -4.142  97.143  32.076  1.00 40.89      S   O
ATOM  4469  OH2 TIP S 492      8.626 110.626  48.140  1.00 38.81      S   O
ATOM  4470  OH2 TIP S 493     10.344  52.396  54.552  1.00 40.72      S   O
ATOM  4471  OH2 TIP S 504     -6.927  90.936  52.736  1.00 32.58      S   O
ATOM  4472  OH2 TIP S 506     25.842  56.111  26.259  1.00 44.04      S   O
ATOM  4473  OH2 TIP S 511    -18.765  81.021  30.433  1.00 43.07      S   O
ATOM  4474  OH2 TIP S 514    -10.951  95.897  30.634  1.00 35.08      S   O
ATOM  4475  OH2 TIP S 515     18.239  91.555  29.988  1.00 35.01      S   O
ATOM  4476  OH2 TIP S 518     11.487  71.453  37.559  1.00 30.35      S   O
ATOM  4477  OH2 TIP S 519     -5.621  94.181  63.866  1.00 38.29      S   O
ATOM  4478  OH2 TIP S 522    -22.715  82.630  39.313  1.00 37.68      S   O
ATOM  4479  OH2 TIP S 523     13.832  92.634  28.634  1.00 42.35      S   O
ATOM  4480  OH2 TIP S 526     38.684  51.235  34.304  1.00 47.63      S   O
ATOM  4481  OH2 TIP S 528     36.575  81.337  36.652  1.00 30.20      S   O
ATOM  4482  OH2 TIP S 529     19.003  94.626  60.449  1.00 33.39      S   O
ATOM  4483  OH2 TIP S 532     45.213  64.758  44.484  1.00 43.40      S   O
ATOM  4484  OH2 TIP S 548     27.913  76.880  61.466  1.00 39.53      S   O
ATOM  4485  OH2 TIP S 550     -7.794  83.071  55.228  1.00 36.58      S   O
ATOM  4486  OH2 TIP S 551      6.856  87.791  20.410  1.00 45.36      S   O
ATOM  4487  OH2 TIP S 553     20.954  56.587  35.076  1.00 46.06      S   O
ATOM  4488  OH2 TIP S 559      6.709  95.476  37.577  1.00 37.67      S   O
ATOM  4489  OH2 TIP S 561     -5.111  70.585  43.095  1.00 36.29      S   O
ATOM  4490  OH2 TIP S 563     33.592  49.188  39.439  1.00 38.90      S   O
ATOM  4491  OH2 TIP S 567     24.268  93.456  38.866  1.00 41.73      S   O
ATOM  4492  OH2 TIP S 568     38.145  71.373  18.079  1.00 45.93      S   O
ATOM  4493  OH2 TIP S 570     10.042 104.897  57.893  1.00 35.94      S   O
ATOM  4494  OH2 TIP S 579      2.980  71.667  46.083  1.00 31.08      S   O
ATOM  4495  OH2 TIP S 588     42.992  48.494  46.292  1.00 42.53      S   O
ATOM  4496  OH2 TIP S 592      7.979 101.256  62.776  1.00 43.56      S   O
ATOM  4497  OH2 TIP S 596     40.729  51.604  40.374  1.00 44.86      S   O
ATOM  4498  OH2 TIP S 608     22.066  82.819  34.739  1.00 44.19      S   O
ATOM  4499  OH2 TIP S 612     23.253  56.890  32.646  1.00 37.91      S   O
ATOM  4500  OH2 TIP S 613     -4.126  71.281  39.257  1.00 40.53      S   O
ATOM  4501  OH2 TIP S 640     21.624 103.517  40.110  1.00 37.27      S   O
ATOM  4502  OH2 TIP S 648      5.614  70.703  52.258  1.00 52.65      S   O
ATOM  4503  OH2 TIP S 650     43.903  58.744  50.765  1.00 33.40      S   O
ATOM  4504  OH2 TIP S 655     -8.816  78.637  48.006  1.00 40.13      S   O
```

Figure 4ZZZ

```
ATOM  4505  OH2 TIP S 656     -5.358  78.170  23.376  1.00 32.77      S   O
ATOM  4506  OH2 TIP S 657      3.160  70.067  31.591  1.00 35.22      S   O
ATOM  4507  OH2 TIP S 658     25.185  73.553  62.291  1.00 39.81      S   O
END
```

Figure 5A

```
REMARK Created by MOLEMAN V. 991230/7.3 at Tue Dec 10 19:34:52 2002 for kemitl
REMARK MoleMan PDB file
REMARK Created by MOLEMAN V. 961218/7.2.5 at Tue Mar 28 15:09:11 2000 for kemitl
REMARK MoleMan PDB file
REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 1.86 A
REMARK starting r= 0.2208 free_r= 0.2457
REMARK final   r= 0.2055 free_r= 0.2376
REMARK B rmsd for bonded mainchain atoms=  1.483  target= 1.5
REMARK B rmsd for bonded sidechain atoms=  2.506  target= 2.0
REMARK B rmsd for angle mainchain atoms=  2.042  target= 2.0
REMARK B rmsd for angle sidechain atoms=  3.617  target= 2.5
REMARK wa= 1.64705
REMARK rweight=6.377507E-02
REMARK target= mlf  steps= 50
REMARK sg= P2(1)2(1)2(1) a= 61.41 b= 76.31 c= 108.92 alpha= 90 beta= 90 gamma= 90
REMARK parameter file 1  : MSI_CNX_TOPPAR:protein_rep.param
REMARK parameter file 2  : MSI_CNX_TOPPAR:water_rep.param
REMARK parameter file 3  : inh.par
REMARK parameter file 4  : gld.par
REMARK molecular structure file: generate_easy.psf
REMARK input coordinates: bgroup.pdb
REMARK reflection file= muri_1.8.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.86
REMARK initial B-factor correction applied to fobs :
REMARK   B11=  0.497 B22=   1.667 B33= -2.164
REMARK   B12=  0.000 B13=   0.000 B23=  0.000
REMARK B-factor correction applied to coordinate array B:    1.176
REMARK bulk solvent: (Mask) density level= 0.365438 e/A^3, B-factor= 33.2255 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range:    43743 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):  3410 (  7.8 % )
REMARK number of reflections rejected:                          0 (  0.0 % )
REMARK total number of reflections used:                    40333 ( 92.2 % )
REMARK number of reflections in working set:                38313 ( 87.6 % )
REMARK number of reflections in test set:                   2020 (  4.6 % )
REMARK FILENAME="bindividual.pdb"
REMARK DATE:Mar-24-2000  16:16:02      created by user: kemitl
REMARK Written by CNX VERSION:2000
CRYST1  61.410  76.310 108.920 90.00 90.00  90.00 P212121      1
ORIGX1     1.000000 0.000000 0.000000       0.00000
ORIGX2     0.000000 1.000000 0.000000       0.00000
ORIGX3     0.000000 0.000000 1.000000       0.00000
SCALE1     0.016284 0.000000 0.000000       0.00000
SCALE2     0.000000 0.013104 0.000000       0.00000
SCALE3     0.000000 0.000000 0.009181       0.00000
ATOM     1  CB  MET A  1     30.124  48.907  56.585  1.00 22.42     A   C
ATOM     2  CG  MET A  1     30.702  50.302  56.333  1.00 25.22     A   C
ATOM     3  SD  MET A  1     31.489  51.055  57.785  1.00 28.98     A   S
ATOM     4  CE  MET A  1     32.951  49.983  58.010  1.00 26.14     A   C
ATOM     5  C   MET A  1     27.890  49.690  57.412  1.00 19.35     A   C
ATOM     6  O   MET A  1     27.114  49.386  56.503  1.00 20.53     A   O
ATOM     7  N   MET A  1     28.658  47.421  57.925  1.00 18.28     A   N
ATOM     8  CA  MET A  1     29.106  48.829  57.729  1.00 20.61     A   C
ATOM     9  N   LYS A  2     27.729  50.760  58.178  1.00 18.84     A   N
ATOM    10  CA  LYS A  2     26.605  51.666  58.005  1.00 19.29     A   C
```

Figure 5B

```
ATOM   11 CB  LYS A  2     25.834  51.769  59.316  1.00 18.82    A   C
ATOM   12 CG  LYS A  2     24.636  52.702  59.295  1.00 20.09    A   C
ATOM   13 CD  LYS A  2     24.005  52.752  60.674  1.00 22.85    A   C
ATOM   14 CE  LYS A  2     22.697  53.523  60.676  1.00 22.98    A   C
ATOM   15 NZ  LYS A  2     22.078  53.501  62.033  1.00 22.51    A   N
ATOM   16 C   LYS A  2     27.131  53.031  57.588  1.00 17.25    A   C
ATOM   17 O   LYS A  2     27.980  53.616  58.265  1.00 16.44    A   O
ATOM   18 N   ILE A  3     26.630  53.533  56.464  1.00 17.70    A   N
ATOM   19 CA  ILE A  3     27.075  54.824  55.968  1.00 14.65    A   C
ATOM   20 CB  ILE A  3     28.001  54.647  54.738  1.00 16.82    A   C
ATOM   21 CG2 ILE A  3     29.214  53.807  55.121  1.00 17.12    A   C
ATOM   22 CG1 ILE A  3     27.252  53.971  53.593  1.00 17.27    A   C
ATOM   23 CD1 ILE A  3     26.697  54.929  52.583  1.00 20.09    A   C
ATOM   24 C   ILE A  3     25.925  55.758  55.617  1.00 14.64    A   C
ATOM   25 O   ILE A  3     24.752  55.377  55.639  1.00 14.39    A   O
ATOM   26 N   GLY A  4     26.269  57.001  55.322  1.00 13.89    A   N
ATOM   27 CA  GLY A  4     25.244  57.956  54.961  1.00 14.96    A   C
ATOM   28 C   GLY A  4     25.500  58.490  53.569  1.00 13.26    A   C
ATOM   29 O   GLY A  4     26.634  58.453  53.081  1.00 11.89    A   O
ATOM   30 N   VAL A  5     24.439  58.954  52.917  1.00 11.22    A   N
ATOM   31 CA  VAL A  5     24.549  59.541  51.592  1.00 10.79    A   C
ATOM   32 CB  VAL A  5     23.964  58.625  50.500  1.00 14.07    A   C
ATOM   33 CG1 VAL A  5     23.918  59.363  49.169  1.00 12.77    A   C
ATOM   34 CG2 VAL A  5     24.828  57.385  50.352  1.00 12.02    A   C
ATOM   35 C   VAL A  5     23.771  60.848  51.643  1.00 11.63    A   C
ATOM   36 O   VAL A  5     22.596  60.872  52.020  1.00 12.22    A   O
ATOM   37 N   PHE A  6     24.445  61.932  51.287  1.00 11.51    A   N
ATOM   38 CA  PHE A  6     23.848  63.256  51.302  1.00 13.29    A   C
ATOM   39 CB  PHE A  6     24.674  64.182  52.203  1.00 13.43    A   C
ATOM   40 CG  PHE A  6     24.252  65.620  52.143  1.00 14.85    A   C
ATOM   41 CD1 PHE A  6     22.937  65.981  52.418  1.00 16.29    A   C
ATOM   42 CD2 PHE A  6     25.164  66.612  51.800  1.00 15.26    A   C
ATOM   43 CE1 PHE A  6     22.530  67.317  52.350  1.00 17.43    A   C
ATOM   44 CE2 PHE A  6     24.770  67.954  51.728  1.00 17.55    A   C
ATOM   45 CZ  PHE A  6     23.450  68.305  52.003  1.00 18.07    A   C
ATOM   46 C   PHE A  6     23.725  63.887  49.920  1.00 12.87    A   C
ATOM   47 O   PHE A  6     24.641  63.806  49.102  1.00 14.09    A   O
ATOM   48 N   ASP A  7     22.583  64.519  49.674  1.00 11.45    A   N
ATOM   49 CA  ASP A  7     22.331  65.212  48.418  1.00 12.53    A   C
ATOM   50 CB  ASP A  7     21.749  64.263  47.363  1.00 11.52    A   C
ATOM   51 CG  ASP A  7     21.491  64.959  46.035  1.00 10.71    A   C
ATOM   52 OD1 ASP A  7     22.444  65.525  45.457  1.00 12.13    A   O
ATOM   53 OD2 ASP A  7     20.332  64.944  45.571  1.00 11.62    A   O
ATOM   54 C   ASP A  7     21.353  66.350  48.670  1.00 10.34    A   C
ATOM   55 O   ASP A  7     20.714  66.410  49.716  1.00 12.06    A   O
ATOM   56 N   SER A  8     21.245  67.262  47.713  1.00 12.07    A   N
ATOM   57 CA  SER A  8     20.330  68.387  47.856  1.00 12.93    A   C
ATOM   58 CB  SER A  8     20.595  69.417  46.756  1.00 12.10    A   C
ATOM   59 OG  SER A  8     20.364  68.857  45.474  1.00 10.24    A   O
ATOM   60 C   SER A  8     18.874  67.909  47.783  1.00 13.34    A   C
ATOM   61 O   SER A  8     17.957  68.609  48.217  1.00 14.16    A   O
ATOM   62 N   GLY A  9     18.667  66.709  47.250  1.00 13.06    A   N
ATOM   63 CA  GLY A  9     17.319  66.182  47.143  1.00 12.56    A   C
ATOM   64 C   GLY A  9     17.253  64.728  46.721  1.00 13.45    A   C
ATOM   65 O   GLY A  9     17.886  63.861  47.329  1.00 13.56    A   O
ATOM   66 N   VAL A 10     16.484  64.460  45.671  1.00 12.87    A   N
ATOM   67 CA  VAL A 10     16.323  63.104  45.159  1.00 12.62    A   C
ATOM   68 CB  VAL A 10     14.916  62.935  44.552  1.00 12.47    A   C
```

Figure 5C

```
ATOM   69 CG1 VAL A 10    14.715 63.955 43.453 1.00 11.29    A   C
ATOM   70 CG2 VAL A 10    14.720 61.521 44.031 1.00 12.71    A   C
ATOM   71 C   VAL A 10    17.372 62.785 44.095 1.00 12.55    A   C
ATOM   72 O   VAL A 10    17.586 61.624 43.749 1.00 11.19    A   O
ATOM   73 N   GLY A 11    18.020 63.823 43.575 1.00 12.78    A   N
ATOM   74 CA  GLY A 11    19.032 63.623 42.548 1.00 10.57    A   C
ATOM   75 C   GLY A 11    20.039 62.536 42.884 1.00 12.63    A   C
ATOM   76 O   GLY A 11    20.376 61.696 42.035 1.00 12.33    A   O
ATOM   77 N   GLY A 12    20.514 62.560 44.126 1.00 12.27    A   N
ATOM   78 CA  GLY A 12    21.488 61.589 44.597 1.00 13.34    A   C
ATOM   79 C   GLY A 12    21.125 60.142 44.331 1.00 12.55    A   C
ATOM   80 O   GLY A 12    21.963 59.252 44.496 1.00 12.07    A   O
ATOM   81 N   PHE A 13    19.877 59.894 43.938 1.00 11.81    A   N
ATOM   82 CA  PHE A 13    19.447 58.534 43.619 1.00 12.39    A   C
ATOM   83 CB  PHE A 13    18.009 58.515 43.081 1.00 13.67    A   C
ATOM   84 CG  PHE A 13    16.947 58.401 44.148 1.00 13.33    A   C
ATOM   85 CD1 PHE A 13    15.671 57.955 43.816 1.00 14.75    A   C
ATOM   86 CD2 PHE A 13    17.215 58.740 45.470 1.00 13.91    A   C
ATOM   87 CE1 PHE A 13    14.667 57.846 44.790 1.00 18.10    A   C
ATOM   88 CE2 PHE A 13    16.221 58.635 46.454 1.00 15.28    A   C
ATOM   89 CZ  PHE A 13    14.943 58.186 46.112 1.00 13.91    A   C
ATOM   90 C   PHE A 13    20.361 57.940 42.547 1.00 13.92    A   C
ATOM   91 O   PHE A 13    20.630 56.737 42.551 1.00 12.12    A   O
ATOM   92 N   SER A 14    20.827 58.781 41.625 1.00 13.26    A   N
ATOM   93 CA  SER A 14    21.690 58.304 40.547 1.00 13.42    A   C
ATOM   94 CB  SER A 14    21.967 59.423 39.525 1.00 13.96    A   C
ATOM   95 OG  SER A 14    22.695 60.504 40.071 1.00 12.20    A   O
ATOM   96 C   SER A 14    22.992 57.730 41.092 1.00 13.28    A   C
ATOM   97 O   SER A 14    23.559 56.805 40.509 1.00 14.54    A   O
ATOM   98 N   VAL A 15    23.458 58.270 42.214 1.00 10.88    A   N
ATOM   99 CA  VAL A 15    24.674 57.777 42.846 1.00 11.83    A   C
ATOM  100 CB  VAL A 15    25.338 58.859 43.730 1.00 11.43    A   C
ATOM  101 CG1 VAL A 15    26.452 58.243 44.580 1.00 10.44    A   C
ATOM  102 CG2 VAL A 15    25.909 59.960 42.849 1.00 11.65    A   C
ATOM  103 C   VAL A 15    24.333 56.566 43.709 1.00 13.82    A   C
ATOM  104 O   VAL A 15    25.068 55.579 43.727 1.00 13.72    A   O
ATOM  105 N   LEU A 16    23.199 56.635 44.400 1.00 13.39    A   N
ATOM  106 CA  LEU A 16    22.767 55.546 45.264 1.00 14.00    A   C
ATOM  107 CB  LEU A 16    21.479 55.937 45.993 1.00 11.47    A   C
ATOM  108 CG  LEU A 16    20.947 54.898 46.991 1.00 14.59    A   C
ATOM  109 CD1 LEU A 16    22.049 54.511 47.980 1.00 13.56    A   C
ATOM  110 CD2 LEU A 16    19.743 55.477 47.733 1.00 10.24    A   C
ATOM  111 C   LEU A 16    22.562 54.246 44.486 1.00 14.34    A   C
ATOM  112 O   LEU A 16    22.879 53.162 44.980 1.00 13.30    A   O
ATOM  113 N   LYS A 17    22.044 54.356 43.267 1.00 14.05    A   N
ATOM  114 CA  LYS A 17    21.822 53.176 42.438 1.00 16.52    A   C
ATOM  115 CB  LYS A 17    21.229 53.584 41.087 1.00 16.99    A   C
ATOM  116 CG  LYS A 17    21.051 52.424 40.114 1.00 21.73    A   C
ATOM  117 CD  LYS A 17    20.461 52.893 38.802 1.00 24.05    A   C
ATOM  118 CE  LYS A 17    20.298 51.729 37.833 1.00 27.52    A   C
ATOM  119 NZ  LYS A 17    19.805 52.178 36.505 1.00 24.97    A   N
ATOM  120 C   LYS A 17    23.136 52.423 42.220 1.00 17.90    A   C
ATOM  121 O   LYS A 17    23.194 51.193 42.319 1.00 16.07    A   O
ATOM  122 N   SER A 18    24.193 53.171 41.931 1.00 16.04    A   N
ATOM  123 CA  SER A 18    25.508 52.582 41.691 1.00 17.22    A   C
ATOM  124 CB  SER A 18    26.494 53.663 41.248 1.00 16.33    A   C
ATOM  125 OG  SER A 18    26.080 54.255 40.034 1.00 15.13    A   O
ATOM  126 C   SER A 18    26.033 51.900 42.944 1.00 16.33    A   C
```

Figure 5D

```
ATOM   127  O   SER A  18      26.579  50.795  42.885  1.00 14.32      A   O
ATOM   128  N   LEU A  19      25.863  52.577  44.075  1.00 13.38      A   N
ATOM   129  CA  LEU A  19      26.301  52.072  45.367  1.00 14.03      A   C
ATOM   130  CB  LEU A  19      26.009  53.102  46.456  1.00 11.70      A   C
ATOM   131  CG  LEU A  19      26.748  54.435  46.350  1.00 12.66      A   C
ATOM   132  CD1 LEU A  19      26.284  55.365  47.471  1.00 13.24      A   C
ATOM   133  CD2 LEU A  19      28.248  54.185  46.442  1.00 11.34      A   C
ATOM   134  C   LEU A  19      25.605  50.771  45.720  1.00 15.80      A   C
ATOM   135  O   LEU A  19      26.240  49.831  46.195  1.00 14.57      A   O
ATOM   136  N   LEU A  20      24.294  50.727  45.496  1.00 15.82      A   N
ATOM   137  CA  LEU A  20      23.510  49.540  45.793  1.00 18.19      A   C
ATOM   138  CB  LEU A  20      22.026  49.807  45.515  1.00 16.40      A   C
ATOM   139  CG  LEU A  20      21.346  50.798  46.473  1.00 16.62      A   C
ATOM   140  CD1 LEU A  20      19.949  51.156  45.974  1.00 16.53      A   C
ATOM   141  CD2 LEU A  20      21.279  50.176  47.867  1.00 16.65      A   C
ATOM   142  C   LEU A  20      23.983  48.330  44.988  1.00 20.92      A   C
ATOM   143  O   LEU A  20      24.179  47.247  45.538  1.00 20.94      A   O
ATOM   144  N   LYS A  21      24.169  48.511  43.687  1.00 20.60      A   N
ATOM   145  CA  LYS A  21      24.612  47.406  42.847  1.00 22.68      A   C
ATOM   146  CB  LYS A  21      24.656  47.840  41.380  1.00 21.65      A   C
ATOM   147  CG  LYS A  21      24.973  46.699  40.426  1.00 26.15      A   C
ATOM   148  CD  LYS A  21      25.083  47.169  38.988  1.00 29.67      A   C
ATOM   149  CE  LYS A  21      25.506  46.017  38.078  1.00 34.31      A   C
ATOM   150  NZ  LYS A  21      25.776  46.469  36.684  1.00 32.80      A   N
ATOM   151  C   LYS A  21      25.978  46.863  43.263  1.00 21.58      A   C
ATOM   152  O   LYS A  21      26.214  45.654  43.208  1.00 23.12      A   O
ATOM   153  N   ALA A  22      26.868  47.753  43.692  1.00 19.68      A   N
ATOM   154  CA  ALA A  22      28.216  47.360  44.093  1.00 19.96      A   C
ATOM   155  CB  ALA A  22      29.131  48.585  44.080  1.00 14.81      A   C
ATOM   156  C   ALA A  22      28.317  46.635  45.446  1.00 20.35      A   C
ATOM   157  O   ALA A  22      29.402  46.199  45.839  1.00 21.92      A   O
ATOM   158  N   ARG A  23      27.198  46.509  46.154  1.00 20.50      A   N
ATOM   159  CA  ARG A  23      27.187  45.821  47.444  1.00 21.19      A   C
ATOM   160  CB  ARG A  23      27.205  44.307  47.230  1.00 23.64      A   C
ATOM   161  CG  ARG A  23      25.965  43.756  46.553  1.00 24.47      A   C
ATOM   162  CD  ARG A  23      26.093  42.252  46.372  1.00 30.28      A   C
ATOM   163  NE  ARG A  23      26.418  41.582  47.630  1.00 30.56      A   N
ATOM   164  CZ  ARG A  23      26.768  40.302  47.727  1.00 32.70      A   C
ATOM   165  NH1 ARG A  23      26.838  39.549  46.636  1.00 32.50      A   N
ATOM   166  NH2 ARG A  23      27.054  39.776  48.914  1.00 28.66      A   N
ATOM   167  C   ARG A  23      28.379  46.216  48.302  1.00 21.73      A   C
ATOM   168  O   ARG A  23      29.149  45.365  48.759  1.00 20.27      A   O
ATOM   169  N   LEU A  24      28.522  47.512  48.527  1.00 17.52      A   N
ATOM   170  CA  LEU A  24      29.624  48.018  49.317  1.00 21.03      A   C
ATOM   171  CB  LEU A  24      30.080  49.366  48.757  1.00 20.25      A   C
ATOM   172  CG  LEU A  24      30.478  49.366  47.282  1.00 22.97      A   C
ATOM   173  CD1 LEU A  24      30.723  50.797  46.810  1.00 22.12      A   C
ATOM   174  CD2 LEU A  24      31.723  48.510  47.094  1.00 21.35      A   C
ATOM   175  C   LEU A  24      29.239  48.184  50.776  1.00 21.90      A   C
ATOM   176  O   LEU A  24      30.079  48.032  51.663  1.00 23.97      A   O
ATOM   177  N   PHE A  25      27.968  48.483  51.028  1.00 20.73      A   N
ATOM   178  CA  PHE A  25      27.517  48.710  52.396  1.00 21.16      A   C
ATOM   179  CB  PHE A  25      27.290  50.207  52.609  1.00 19.75      A   C
ATOM   180  CG  PHE A  25      28.416  51.062  52.101  1.00 19.70      A   C
ATOM   181  CD1 PHE A  25      28.249  51.854  50.967  1.00 20.65      A   C
ATOM   182  CD2 PHE A  25      29.648  51.065  52.748  1.00 19.59      A   C
ATOM   183  CE1 PHE A  25      29.294  52.641  50.483  1.00 20.02      A   C
ATOM   184  CE2 PHE A  25      30.701  51.846  52.276  1.00 20.92      A   C
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Figure 5E

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ATOM   185 CZ  PHE A 25    30.522  52.639  51.137  1.00 19.72    A   C
ATOM   186 C   PHE A 25    26.259  47.940  52.773  1.00 18.19    A   C
ATOM   187 O   PHE A 25    25.387  47.718  51.945  1.00 20.08    A   O
ATOM   188 N   ASP A 26    26.174  47.562  54.044  1.00 19.15    A   N
ATOM   189 CA  ASP A 26    25.049  46.793  54.569  1.00 19.40    A   C
ATOM   190 CB  ASP A 26    25.524  45.978  55.768  1.00 21.39    A   C
ATOM   191 CG  ASP A 26    26.764  45.166  55.455  1.00 23.64    A   C
ATOM   192 OD1 ASP A 26    26.632  44.118  54.794  1.00 23.32    A   O
ATOM   193 OD2 ASP A 26    27.875  45.587  55.852  1.00 28.55    A   O
ATOM   194 C   ASP A 26    23.864  47.662  54.978  1.00 18.82    A   C
ATOM   195 O   ASP A 26    22.727  47.196  55.034  1.00 19.35    A   O
ATOM   196 N   GLU A 27    24.132  48.926  55.273  1.00 17.90    A   N
ATOM   197 CA  GLU A 27    23.067  49.840  55.671  1.00 17.07    A   C
ATOM   198 CB  GLU A 27    22.892  49.826  57.187  1.00 17.71    A   C
ATOM   199 CG  GLU A 27    21.646  50.550  57.663  1.00 24.75    A   C
ATOM   200 CD  GLU A 27    21.322  50.279  59.127  1.00 28.18    A   C
ATOM   201 OE1 GLU A 27    20.326  50.846  59.620  1.00 31.23    A   O
ATOM   202 OE2 GLU A 27    22.054  49.500  59.782  1.00 27.47    A   O
ATOM   203 C   GLU A 27    23.393  51.246  55.197  1.00 16.15    A   C
ATOM   204 O   GLU A 27    24.524  51.723  55.346  1.00 14.85    A   O
ATOM   205 N   ILE A 28    22.393  51.910  54.633  1.00 14.40    A   N
ATOM   206 CA  ILE A 28    22.577  53.257  54.118  1.00 12.75    A   C
ATOM   207 CB  ILE A 28    22.574  53.257  52.582  1.00 13.36    A   C
ATOM   208 CG2 ILE A 28    22.678  54.689  52.056  1.00  9.46    A   C
ATOM   209 CG1 ILE A 28    23.736  52.409  52.059  1.00 12.29    A   C
ATOM   210 CD1 ILE A 28    23.699  52.211  50.552  1.00 16.70    A   C
ATOM   211 C   ILE A 28    21.477  54.193  54.592  1.00 13.60    A   C
ATOM   212 O   ILE A 28    20.296  53.854  54.545  1.00 13.62    A   O
ATOM   213 N   ILE A 29    21.879  55.367  55.059  1.00 12.74    A   N
ATOM   214 CA  ILE A 29    20.928  56.375  55.507  1.00 14.14    A   C
ATOM   215 CB  ILE A 29    21.293  56.944  56.893  1.00 13.73    A   C
ATOM   216 CG2 ILE A 29    20.241  57.957  57.324  1.00 15.30    A   C
ATOM   217 CG1 ILE A 29    21.398  55.814  57.929  1.00 15.05    A   C
ATOM   218 CD1 ILE A 29    20.107  55.035  58.145  1.00 14.22    A   C
ATOM   219 C   ILE A 29    21.039  57.489  54.472  1.00 14.66    A   C
ATOM   220 O   ILE A 29    22.056  58.183  54.404  1.00 13.06    A   O
ATOM   221 N   TYR A 30    20.007  57.629  53.648  1.00 12.88    A   N
ATOM   222 CA  TYR A 30    19.987  58.649  52.609  1.00 14.23    A   C
ATOM   223 CB  TYR A 30    19.221  58.133  51.389  1.00 12.46    A   C
ATOM   224 CG  TYR A 30    19.221  59.075  50.205  1.00 15.02    A   C
ATOM   225 CD1 TYR A 30    20.155  58.933  49.178  1.00 12.86    A   C
ATOM   226 CE1 TYR A 30    20.171  59.803  48.088  1.00 12.85    A   C
ATOM   227 CD2 TYR A 30    18.298  60.119  50.117  1.00 15.96    A   C
ATOM   228 CE2 TYR A 30    18.304  60.996  49.034  1.00 15.05    A   C
ATOM   229 CZ  TYR A 30    19.243  60.831  48.023  1.00 14.12    A   C
ATOM   230 OH  TYR A 30    19.248  61.681  46.948  1.00 11.65    A   O
ATOM   231 C   TYR A 30    19.293  59.902  53.139  1.00 15.46    A   C
ATOM   232 O   TYR A 30    18.211  59.815  53.725  1.00 14.07    A   O
ATOM   233 N   TYR A 31    19.909  61.062  52.934  1.00 14.03    A   N
ATOM   234 CA  TYR A 31    19.297  62.312  53.370  1.00 14.37    A   C
ATOM   235 CB  TYR A 31    20.007  62.882  54.601  1.00 13.42    A   C
ATOM   236 CG  TYR A 31    19.441  64.216  55.045  1.00 13.73    A   C
ATOM   237 CD1 TYR A 31    18.150  64.307  55.559  1.00 15.42    A   C
ATOM   238 CE1 TYR A 31    17.616  65.532  55.962  1.00 18.80    A   C
ATOM   239 CD2 TYR A 31    20.191  65.389  54.940  1.00 15.22    A   C
ATOM   240 CE2 TYR A 31    19.665  66.625  55.335  1.00 19.27    A   C
ATOM   241 CZ  TYR A 31    18.376  66.686  55.847  1.00 20.56    A   C
ATOM   242 OH  TYR A 31    17.840  67.894  56.250  1.00 21.50    A   O
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Figure 5F

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ATOM   243  C  TYR A  31     19.321  63.355  52.257  1.00 13.94    A   C
ATOM   244  O  TYR A  31     20.383  63.704  51.743  1.00 12.53    A   O
ATOM   245  N  GLY A  32     18.139  63.836  51.876  1.00 14.52    A   N
ATOM   246  CA GLY A  32     18.052  64.855  50.846  1.00 11.09    A   C
ATOM   247  C  GLY A  32     17.502  66.137  51.445  1.00 14.21    A   C
ATOM   248  O  GLY A  32     16.474  66.105  52.120  1.00 13.16    A   O
ATOM   249  N  ASP A  33     18.178  67.261  51.217  1.00 11.82    A   N
ATOM   250  CA ASP A  33     17.728  68.550  51.754  1.00 12.90    A   C
ATOM   251  CB ASP A  33     18.934  69.474  51.926  1.00 11.25    A   C
ATOM   252  CG ASP A  33     18.576  70.788  52.587  1.00 11.81    A   C
ATOM   253  OD1 ASP A  33     17.562  70.842  53.309  1.00 14.26    A   O
ATOM   254  OD2 ASP A  33     19.326  71.757  52.394  1.00 11.68    A   O
ATOM   255  C  ASP A  33     16.703  69.145  50.783  1.00 13.65    A   C
ATOM   256  O  ASP A  33     16.824  70.285  50.324  1.00 12.95    A   O
ATOM   257  N  SER A  34     15.693  68.333  50.486  1.00 13.72    A   N
ATOM   258  CA SER A  34     14.630  68.658  49.543  1.00 14.78    A   C
ATOM   259  CB SER A  34     13.602  67.527  49.539  1.00 13.92    A   C
ATOM   260  OG SER A  34     14.230  66.294  49.232  1.00 21.22    A   O
ATOM   261  C  SER A  34     13.914  69.980  49.751  1.00 16.62    A   C
ATOM   262  O  SER A  34     13.379  70.554  48.799  1.00 14.31    A   O
ATOM   263  N  ALA A  35     13.889  70.461  50.990  1.00 13.83    A   N
ATOM   264  CA ALA A  35     13.216  71.717  51.282  1.00 14.72    A   C
ATOM   265  CB ALA A  35     13.037  71.875  52.790  1.00 12.61    A   C
ATOM   266  C  ALA A  35     13.982  72.908  50.717  1.00 15.06    A   C
ATOM   267  O  ALA A  35     13.417  73.989  50.538  1.00 17.76    A   O
ATOM   268  N  ARG A  36     15.262  72.713  50.420  1.00 15.20    A   N
ATOM   269  CA ARG A  36     16.076  73.804  49.902  1.00 15.09    A   C
ATOM   270  CB ARG A  36     17.175  74.128  50.918  1.00 14.65    A   C
ATOM   271  CG ARG A  36     16.585  74.462  52.284  1.00 13.95    A   C
ATOM   272  CD ARG A  36     17.602  75.018  53.255  1.00 15.98    A   C
ATOM   273  NE ARG A  36     18.579  74.020  53.681  1.00 14.55    A   N
ATOM   274  CZ ARG A  36     19.333  74.141  54.769  1.00 19.35    A   C
ATOM   275  NH1 ARG A  36     19.217  75.221  55.537  1.00 16.64    A   N
ATOM   276  NH2 ARG A  36     20.201  73.187  55.093  1.00 16.02    A   N
ATOM   277  C  ARG A  36     16.668  73.578  48.511  1.00 15.81    A   C
ATOM   278  O  ARG A  36     17.422  74.409  48.002  1.00 15.67    A   O
ATOM   279  N  VAL A  37     16.319  72.461  47.888  1.00 15.48    A   N
ATOM   280  CA VAL A  37     16.821  72.168  46.552  1.00 13.76    A   C
ATOM   281  CB VAL A  37     16.374  70.746  46.115  1.00 14.93    A   C
ATOM   282  CG1 VAL A  37     14.877  70.727  45.851  1.00 14.99    A   C
ATOM   283  CG2 VAL A  37     17.174  70.280  44.898  1.00 14.00    A   C
ATOM   284  C  VAL A  37     16.246  73.243  45.617  1.00 11.66    A   C
ATOM   285  O  VAL A  37     15.112  73.697  45.805  1.00 11.22    A   O
ATOM   286  N  PRO A  38     17.011  73.662  44.596  1.00 12.05    A   N
ATOM   287  CD PRO A  38     16.485  74.565  43.553  1.00 12.17    A   C
ATOM   288  CA PRO A  38     18.356  73.214  44.244  1.00 13.67    A   C
ATOM   289  CB PRO A  38     18.368  73.384  42.736  1.00 14.66    A   C
ATOM   290  CG PRO A  38     17.655  74.698  42.588  1.00 12.08    A   C
ATOM   291  C  PRO A  38     19.486  74.000  44.898  1.00 15.15    A   C
ATOM   292  O  PRO A  38     19.297  75.129  45.370  1.00 12.96    A   O
ATOM   293  N  TYR A  39     20.664  73.382  44.900  1.00 11.07    A   N
ATOM   294  CA TYR A  39     21.885  73.974  45.442  1.00 13.74    A   C
ATOM   295  CB TYR A  39     22.796  72.893  46.040  1.00 11.65    A   C
ATOM   296  CG TYR A  39     22.461  72.394  47.428  1.00 12.17    A   C
ATOM   297  CD1 TYR A  39     21.229  72.663  48.031  1.00 13.42    A   C
ATOM   298  CE1 TYR A  39     20.932  72.177  49.312  1.00 12.82    A   C
ATOM   299  CD2 TYR A  39     23.387  71.625  48.137  1.00 14.92    A   C
ATOM   300  CE2 TYR A  39     23.103  71.137  49.406  1.00 15.33    A   C
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Figure 5G

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ATOM   301 CZ  TYR A 39     21.878  71.414  49.992  1.00 13.34    A   C
ATOM   302 OH  TYR A 39     21.624  70.941  51.260  1.00 13.24    A   O
ATOM   303 C   TYR A 39     22.654  74.640  44.300  1.00 11.74    A   C
ATOM   304 O   TYR A 39     23.323  75.652  44.494  1.00 14.92    A   O
ATOM   305 N   GLY A 40     22.551  74.049  43.112  1.00 14.63    A   N
ATOM   306 CA  GLY A 40     23.269  74.529  41.939  1.00 12.47    A   C
ATOM   307 C   GLY A 40     23.196  75.993  41.544  1.00 14.09    A   C
ATOM   308 O   GLY A 40     24.093  76.502  40.871  1.00 12.63    A   O
ATOM   309 N   THR A 41     22.141  76.683  41.952  1.00 13.06    A   N
ATOM   310 CA  THR A 41     22.001  78.086  41.585  1.00 17.35    A   C
ATOM   311 CB  THR A 41     20.552  78.400  41.219  1.00 18.12    A   C
ATOM   312 OG1 THR A 41     19.713  78.078  42.332  1.00 22.00    A   O
ATOM   313 CG2 THR A 41     20.115  77.580  40.009  1.00 22.83    A   C
ATOM   314 C   THR A 41     22.416  79.020  42.712  1.00 16.33    A   C
ATOM   315 O   THR A 41     22.266  80.240  42.600  1.00 17.71    A   O
ATOM   316 N   LYS A 42     22.953  78.460  43.787  1.00 14.75    A   N
ATOM   317 CA  LYS A 42     23.331  79.281  44.922  1.00 13.75    A   C
ATOM   318 CB  LYS A 42     22.653  78.721  46.174  1.00 14.86    A   C
ATOM   319 CG  LYS A 42     21.139  78.899  46.078  1.00 14.53    A   C
ATOM   320 CD  LYS A 42     20.342  77.857  46.842  1.00 14.88    A   C
ATOM   321 CE  LYS A 42     18.898  77.878  46.349  1.00 13.95    A   C
ATOM   322 NZ  LYS A 42     17.995  76.929  47.073  1.00 12.60    A   N
ATOM   323 C   LYS A 42     24.824  79.496  45.119  1.00 16.57    A   C
ATOM   324 O   LYS A 42     25.647  78.943  44.391  1.00 14.82    A   O
ATOM   325 N   ASP A 43     25.157  80.329  46.099  1.00 17.21    A   N
ATOM   326 CA  ASP A 43     26.539  80.689  46.390  1.00 19.06    A   C
ATOM   327 CB  ASP A 43     26.567  82.117  46.932  1.00 20.48    A   C
ATOM   328 CG  ASP A 43     25.808  82.245  48.228  1.00 21.34    A   C
ATOM   329 OD1 ASP A 43     26.458  82.356  49.287  1.00 19.30    A   O
ATOM   330 OD2 ASP A 43     24.557  82.210  48.190  1.00 23.52    A   O
ATOM   331 C   ASP A 43     27.260  79.763  47.371  1.00 19.43    A   C
ATOM   332 O   ASP A 43     26.634  79.034  48.141  1.00 18.30    A   O
ATOM   333 N   PRO A 44     28.604  79.789  47.346  1.00 21.23    A   N
ATOM   334 CD  PRO A 44     29.401  80.567  46.377  1.00 20.65    A   C
ATOM   335 CA  PRO A 44     29.482  78.984  48.202  1.00 20.54    A   C
ATOM   336 CB  PRO A 44     30.866  79.543  47.886  1.00 20.91    A   C
ATOM   337 CG  PRO A 44     30.749  79.881  46.440  1.00 20.03    A   C
ATOM   338 C   PRO A 44     29.165  79.051  49.691  1.00 21.08    A   C
ATOM   339 O   PRO A 44     29.078  78.020  50.362  1.00 22.03    A   O
ATOM   340 N   THR A 45     28.999  80.266  50.207  1.00 20.06    A   N
ATOM   341 CA  THR A 45     28.707  80.453  51.622  1.00 19.83    A   C
ATOM   342 CB  THR A 45     28.523  81.953  51.961  1.00 22.19    A   C
ATOM   343 OG1 THR A 45     29.734  82.659  51.667  1.00 22.93    A   O
ATOM   344 CG2 THR A 45     28.180  82.135  53.429  1.00 21.29    A   C
ATOM   345 C   THR A 45     27.453  79.697  52.027  1.00 18.90    A   C
ATOM   346 O   THR A 45     27.448  78.950  53.007  1.00 16.82    A   O
ATOM   347 N   THR A 46     26.386  79.893  51.263  1.00 17.42    A   N
ATOM   348 CA  THR A 46     25.125  79.235  51.546  1.00 17.81    A   C
ATOM   349 CB  THR A 46     24.039  79.671  50.542  1.00 16.98    A   C
ATOM   350 OG1 THR A 46     23.835  81.087  50.636  1.00 17.53    A   O
ATOM   351 CG2 THR A 46     22.737  78.971  50.839  1.00 19.05    A   C
ATOM   352 C   THR A 46     25.265  77.719  51.484  1.00 17.51    A   C
ATOM   353 O   THR A 46     24.766  77.004  52.355  1.00 18.78    A   O
ATOM   354 N   ILE A 47     25.945  77.236  50.452  1.00 17.91    A   N
ATOM   355 CA  ILE A 47     26.134  75.803  50.265  1.00 20.81    A   C
ATOM   356 CB  ILE A 47     26.822  75.513  48.912  1.00 20.52    A   C
ATOM   357 CG2 ILE A 47     26.934  74.002  48.678  1.00 18.34    A   C
ATOM   358 CG1 ILE A 47     26.004  76.143  47.783  1.00 23.35    A   C
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Figure 5H

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ATOM   359 CD1 ILE A 47    24.523  75.792  47.826  1.00 23.82    A   C
ATOM   360 C   ILE A 47    26.935  75.170  51.398  1.00 19.27    A   C
ATOM   361 O   ILE A 47    26.568  74.111  51.905  1.00 21.96    A   O
ATOM   362 N   LYS A 48    28.018  75.818  51.805  1.00 21.30    A   N
ATOM   363 CA  LYS A 48    28.834  75.292  52.890  1.00 20.85    A   C
ATOM   364 CB  LYS A 48    30.032  76.203  53.151  1.00 22.83    A   C
ATOM   365 CG  LYS A 48    31.094  76.059  52.091  1.00 27.64    A   C
ATOM   366 CD  LYS A 48    32.380  76.794  52.444  1.00 31.38    A   C
ATOM   367 CE  LYS A 48    32.246  78.287  52.245  1.00 32.58    A   C
ATOM   368 NZ  LYS A 48    33.567  78.966  52.404  1.00 35.58    A   N
ATOM   369 C   LYS A 48    28.029  75.101  54.163  1.00 21.38    A   C
ATOM   370 O   LYS A 48    28.141  74.061  54.814  1.00 20.76    A   O
ATOM   371 N   GLN A 49    27.211  76.091  54.520  1.00 19.20    A   N
ATOM   372 CA  GLN A 49    26.395  75.963  55.716  1.00 19.40    A   C
ATOM   373 CB  GLN A 49    25.619  77.256  56.005  1.00 19.30    A   C
ATOM   374 CG  GLN A 49    24.776  77.203  57.286  1.00 22.44    A   C
ATOM   375 CD  GLN A 49    25.581  76.812  58.525  1.00 20.73    A   C
ATOM   376 OE1 GLN A 49    26.740  77.192  58.667  1.00 22.79    A   O
ATOM   377 NE2 GLN A 49    24.958  76.068  59.433  1.00 22.60    A   N
ATOM   378 C   GLN A 49    25.423  74.803  55.553  1.00 18.14    A   C
ATOM   379 O   GLN A 49    25.159  74.074  56.510  1.00 19.87    A   O
ATOM   380 N   PHE A 50    24.882  74.631  54.348  1.00 17.65    A   N
ATOM   381 CA  PHE A 50    23.960  73.521  54.112  1.00 17.56    A   C
ATOM   382 CB  PHE A 50    23.461  73.510  52.659  1.00 17.20    A   C
ATOM   383 CG  PHE A 50    22.478  74.604  52.331  1.00 18.53    A   C
ATOM   384 CD1 PHE A 50    21.961  75.433  53.323  1.00 18.95    A   C
ATOM   385 CD2 PHE A 50    22.041  74.780  51.022  1.00 20.21    A   C
ATOM   386 CE1 PHE A 50    21.023  76.418  53.022  1.00 19.32    A   C
ATOM   387 CE2 PHE A 50    21.101  75.763  50.709  1.00 22.48    A   C
ATOM   388 CZ  PHE A 50    20.592  76.583  51.716  1.00 21.15    A   C
ATOM   389 C   PHE A 50    24.706  72.217  54.401  1.00 15.70    A   C
ATOM   390 O   PHE A 50    24.178  71.311  55.048  1.00 15.38    A   O
ATOM   391 N   GLY A 51    25.945  72.143  53.922  1.00 18.19    A   N
ATOM   392 CA  GLY A 51    26.760  70.959  54.126  1.00 19.41    A   C
ATOM   393 C   GLY A 51    27.006  70.667  55.592  1.00 20.96    A   C
ATOM   394 O   GLY A 51    26.964  69.514  56.026  1.00 20.04    A   O
ATOM   395 N   LEU A 52    27.261  71.716  56.368  1.00 22.33    A   N
ATOM   396 CA  LEU A 52    27.508  71.542  57.791  1.00 22.23    A   C
ATOM   397 CB  LEU A 52    27.995  72.855  58.412  1.00 24.46    A   C
ATOM   398 CG  LEU A 52    29.385  73.328  57.980  1.00 25.92    A   C
ATOM   399 CD1 LEU A 52    29.734  74.618  58.719  1.00 28.98    A   C
ATOM   400 CD2 LEU A 52    30.423  72.249  58.293  1.00 27.40    A   C
ATOM   401 C   LEU A 52    26.246  71.063  58.493  1.00 21.84    A   C
ATOM   402 O   LEU A 52    26.294  70.180  59.344  1.00 21.12    A   O
ATOM   403 N   GLU A 53    25.107  71.635  58.124  1.00 20.72    A   N
ATOM   404 CA  GLU A 53    23.852  71.237  58.736  1.00 20.40    A   C
ATOM   405 CB  GLU A 53    22.731  72.185  58.294  1.00 21.74    A   C
ATOM   406 CG  GLU A 53    22.655  73.438  59.159  1.00 21.95    A   C
ATOM   407 CD  GLU A 53    21.839  74.551  58.536  1.00 23.86    A   C
ATOM   408 OE1 GLU A 53    20.797  74.260  57.906  1.00 23.19    A   O
ATOM   409 OE2 GLU A 53    22.238  75.727  58.685  1.00 24.44    A   O
ATOM   410 C   GLU A 53    23.514  69.789  58.405  1.00 19.46    A   C
ATOM   411 O   GLU A 53    22.813  69.122  59.160  1.00 22.12    A   O
ATOM   412 N   ALA A 54    24.022  69.295  57.282  1.00 20.85    A   N
ATOM   413 CA  ALA A 54    23.760  67.910  56.905  1.00 18.16    A   C
ATOM   414 CB  ALA A 54    24.252  67.647  55.498  1.00 16.88    A   C
ATOM   415 C   ALA A 54    24.474  66.997  57.899  1.00 18.85    A   C
ATOM   416 O   ALA A 54    23.953  65.944  58.280  1.00 18.10    A   O
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Figure 5I

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ATOM   417 N   LEU A 55    25.670 67.408 58.313 1.00 19.45    A   N
ATOM   418 CA  LEU A 55    26.442 66.639 59.281 1.00 19.66    A   C
ATOM   419 CB  LEU A 55    27.775 67.329 59.590 1.00 21.26    A   C
ATOM   420 CG  LEU A 55    28.782 67.408 58.442 1.00 22.31    A   C
ATOM   421 CD1 LEU A 55    30.070 68.042 58.935 1.00 21.17    A   C
ATOM   422 CD2 LEU A 55    29.055 66.008 57.898 1.00 22.77    A   C
ATOM   423 C   LEU A 55    25.626 66.504 60.556 1.00 21.84    A   C
ATOM   424 O   LEU A 55    25.589 65.437 61.166 1.00 20.58    A   O
ATOM   425 N   ASP A 56    24.959 67.584 60.953 1.00 21.85    A   N
ATOM   426 CA  ASP A 56    24.147 67.543 62.157 1.00 22.53    A   C
ATOM   427 CB  ASP A 56    23.506 68.904 62.437 1.00 25.87    A   C
ATOM   428 CG  ASP A 56    24.530 69.986 62.715 1.00 29.28    A   C
ATOM   429 OD1 ASP A 56    25.636 69.651 63.190 1.00 31.33    A   O
ATOM   430 OD2 ASP A 56    24.226 71.172 62.473 1.00 32.07    A   O
ATOM   431 C   ASP A 56    23.062 66.492 62.023 1.00 22.75    A   C
ATOM   432 O   ASP A 56    22.777 65.762 62.974 1.00 22.74    A   O
ATOM   433 N   PHE A 57    22.459 66.403 60.841 1.00 20.21    A   N
ATOM   434 CA  PHE A 57    21.404 65.422 60.633 1.00 21.09    A   C
ATOM   435 CB  PHE A 57    20.831 65.497 59.215 1.00 21.92    A   C
ATOM   436 CG  PHE A 57    19.915 64.352 58.893 1.00 21.43    A   C
ATOM   437 CD1 PHE A 57    18.609 64.336 59.370 1.00 22.87    A   C
ATOM   438 CD2 PHE A 57    20.393 63.233 58.214 1.00 20.64    A   C
ATOM   439 CE1 PHE A 57    17.792 63.218 59.184 1.00 20.01    A   C
ATOM   440 CE2 PHE A 57    19.589 62.112 58.024 1.00 21.14    A   C
ATOM   441 CZ  PHE A 57    18.286 62.104 58.512 1.00 23.52    A   C
ATOM   442 C   PHE A 57    21.873 63.991 60.864 1.00 18.61    A   C
ATOM   443 O   PHE A 57    21.148 63.181 61.441 1.00 20.52    A   O
ATOM   444 N   PHE A 58    23.081 63.679 60.408 1.00 19.51    A   N
ATOM   445 CA  PHE A 58    23.615 62.324 60.532 1.00 21.64    A   C
ATOM   446 CB  PHE A 58    24.701 62.097 59.478 1.00 18.15    A   C
ATOM   447 CG  PHE A 58    24.181 62.018 58.072 1.00 17.07    A   C
ATOM   448 CD1 PHE A 58    24.380 63.072 57.180 1.00 15.61    A   C
ATOM   449 CD2 PHE A 58    23.508 60.878 57.628 1.00 16.58    A   C
ATOM   450 CE1 PHE A 58    23.920 62.993 55.868 1.00 16.17    A   C
ATOM   451 CE2 PHE A 58    23.044 60.790 56.318 1.00 20.24    A   C
ATOM   452 CZ  PHE A 58    23.251 61.850 55.436 1.00 14.25    A   C
ATOM   453 C   PHE A 58    24.164 61.894 61.896 1.00 24.25    A   C
ATOM   454 O   PHE A 58    24.323 60.697 62.147 1.00 24.91    A   O
ATOM   455 N   LYS A 59    24.449 62.850 62.774 1.00 26.87    A   N
ATOM   456 CA  LYS A 59    25.014 62.528 64.087 1.00 28.83    A   C
ATOM   457 CB  LYS A 59    25.116 63.800 64.931 1.00 31.02    A   C
ATOM   458 CG  LYS A 59    26.127 64.792 64.374 1.00 33.56    A   C
ATOM   459 CD  LYS A 59    26.237 66.047 65.221 1.00 37.86    A   C
ATOM   460 CE  LYS A 59    27.270 67.000 64.632 1.00 38.94    A   C
ATOM   461 NZ  LYS A 59    27.433 68.240 65.443 1.00 41.75    A   N
ATOM   462 C   LYS A 59    24.312 61.419 64.879 1.00 28.21    A   C
ATOM   463 O   LYS A 59    24.973 60.541 65.439 1.00 28.12    A   O
ATOM   464 N   PRO A 60    22.969 61.437 64.933 1.00 27.85    A   N
ATOM   465 CD  PRO A 60    22.061 62.472 64.412 1.00 27.44    A   C
ATOM   466 CA  PRO A 60    22.219 60.409 65.671 1.00 26.21    A   C
ATOM   467 CB  PRO A 60    20.791 60.962 65.691 1.00 28.29    A   C
ATOM   468 CG  PRO A 60    20.961 62.446 65.419 1.00 29.74    A   C
ATOM   469 C   PRO A 60    22.264 59.040 64.994 1.00 25.09    A   C
ATOM   470 O   PRO A 60    22.116 58.004 65.640 1.00 24.61    A   O
ATOM   471 N   HIS A 61    22.469 59.045 63.682 1.00 24.30    A   N
ATOM   472 CA  HIS A 61    22.489 57.815 62.906 1.00 23.28    A   C
ATOM   473 CB  HIS A 61    22.210 58.148 61.445 1.00 23.75    A   C
ATOM   474 CG  HIS A 61    20.813 58.616 61.202 1.00 23.81    A   C
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Figure 5J

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ATOM   475 CD2 HIS A 61     20.307  59.858  61.017  1.00 24.28    A   C
ATOM   476 ND1 HIS A 61     19.738  57.753  61.163  1.00 21.57    A   N
ATOM   477 CE1 HIS A 61     18.631  58.443  60.963  1.00 21.88    A   C
ATOM   478 NE2 HIS A 61     18.948  59.723  60.871  1.00 24.37    A   N
ATOM   479 C   HIS A 61    23.754  56.979  63.012  1.00 23.45    A   C
ATOM   480 O   HIS A 61    23.812  55.879  62.475  1.00 23.17    A   O
ATOM   481 N   GLU A 62    24.752  57.497  63.718  1.00 26.52    A   N
ATOM   482 CA  GLU A 62     26.030  56.811  63.892  1.00 27.77    A   C
ATOM   483 CB  GLU A 62     25.944  55.818  65.062  1.00 33.97    A   C
ATOM   484 CG  GLU A 62     24.861  54.754  64.943  1.00 37.16    A   C
ATOM   485 CD  GLU A 62     24.468  54.176  66.292  1.00 40.46    A   C
ATOM   486 OE1 GLU A 62     25.367  53.907  67.117  1.00 41.12    A   O
ATOM   487 OE2 GLU A 62     23.255  53.983  66.525  1.00 42.43    A   O
ATOM   488 C   GLU A 62    26.545  56.118  62.626  1.00 26.21    A   C
ATOM   489 O   GLU A 62    26.699  54.897  62.579  1.00 26.16    A   O
ATOM   490 N   ILE A 63    26.798  56.913  61.591  1.00 22.24    A   N
ATOM   491 CA  ILE A 63     27.333  56.385  60.338  1.00 21.10    A   C
ATOM   492 CB  ILE A 63     26.904  57.246  59.124  1.00 19.78    A   C
ATOM   493 CG2 ILE A 63     25.416  57.065  58.859  1.00 15.78    A   C
ATOM   494 CG1 ILE A 63     27.224  58.718  59.388  1.00 16.88    A   C
ATOM   495 CD1 ILE A 63     27.000  59.636  58.189  1.00 18.48    A   C
ATOM   496 C   ILE A 63    28.853  56.420  60.483  1.00 18.95    A   C
ATOM   497 O   ILE A 63    29.385  57.182  61.293  1.00 19.85    A   O
ATOM   498 N   GLU A 64    29.553  55.593  59.718  1.00 19.95    A   N
ATOM   499 CA  GLU A 64     31.008  55.561  59.804  1.00 19.49    A   C
ATOM   500 CB  GLU A 64     31.492  54.118  59.926  1.00 22.43    A   C
ATOM   501 CG  GLU A 64     31.139  53.498  61.268  1.00 26.80    A   C
ATOM   502 CD  GLU A 64     31.762  52.136  61.452  1.00 29.61    A   C
ATOM   503 OE1 GLU A 64     33.012  52.044  61.421  1.00 31.41    A   O
ATOM   504 OE2 GLU A 64     31.003  51.160  61.623  1.00 29.53    A   O
ATOM   505 C   GLU A 64    31.684  56.251  58.630  1.00 17.37    A   C
ATOM   506 O   GLU A 64    32.890  56.453  58.631  1.00 16.28    A   O
ATOM   507 N   LEU A 65    30.890  56.615  57.632  1.00 18.28    A   N
ATOM   508 CA  LEU A 65     31.393  57.308  56.456  1.00 17.15    A   C
ATOM   509 CB  LEU A 65     32.035  56.318  55.478  1.00 18.66    A   C
ATOM   510 CG  LEU A 65     32.582  56.903  54.169  1.00 21.47    A   C
ATOM   511 CD1 LEU A 65     33.667  55.991  53.603  1.00 23.00    A   C
ATOM   512 CD2 LEU A 65     31.449  57.086  53.167  1.00 22.69    A   C
ATOM   513 C   LEU A 65    30.230  58.021  55.786  1.00 16.52    A   C
ATOM   514 O   LEU A 65    29.100  57.539  55.813  1.00 14.91    A   O
ATOM   515 N   LEU A 66    30.510  59.180  55.204  1.00 14.90    A   N
ATOM   516 CA  LEU A 66     29.486  59.946  54.526  1.00 14.23    A   C
ATOM   517 CB  LEU A 66     29.264  61.288  55.231  1.00 14.12    A   C
ATOM   518 CG  LEU A 66     28.297  62.240  54.514  1.00 14.20    A   C
ATOM   519 CD1 LEU A 66     26.932  61.586  54.415  1.00 14.73    A   C
ATOM   520 CD2 LEU A 66     28.195  63.562  55.262  1.00 13.86    A   C
ATOM   521 C   LEU A 66    29.864  60.200  53.077  1.00 14.92    A   C
ATOM   522 O   LEU A 66    30.975  60.642  52.773  1.00 14.96    A   O
ATOM   523 N   ILE A 67    28.938  59.886  52.181  1.00 13.46    A   N
ATOM   524 CA  ILE A 67     29.140  60.124  50.766  1.00 12.96    A   C
ATOM   525 CB  ILE A 67     28.641  58.953  49.886  1.00 13.86    A   C
ATOM   526 CG2 ILE A 67     28.617  59.385  48.419  1.00 12.97    A   C
ATOM   527 CG1 ILE A 67     29.541  57.729  50.066  1.00 14.37    A   C
ATOM   528 CD1 ILE A 67     29.105  56.530  49.237  1.00 18.27    A   C
ATOM   529 C   ILE A 67    28.314  61.346  50.406  1.00 12.36    A   C
ATOM   530 O   ILE A 67    27.116  61.420  50.719  1.00 13.82    A   O
ATOM   531 N   VAL A 68    28.964  62.317  49.780  1.00 12.37    A   N
ATOM   532 CA  VAL A 68     28.275  63.516  49.342  1.00 12.34    A   C
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Figure 5K

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ATOM   533 CB  VAL A 68     29.160  64.759  49.466  1.00 10.71    A   C
ATOM   534 CG1 VAL A 68     28.413  65.977  48.916  1.00 10.16    A   C
ATOM   535 CG2 VAL A 68     29.525  64.978  50.927  1.00 11.52    A   C
ATOM   536 C   VAL A 68     28.002  63.222  47.884  1.00 11.20    A   C
ATOM   537 O   VAL A 68     28.885  63.362  47.038  1.00 12.44    A   O
ATOM   538 N   ALA A 69     26.785  62.775  47.602  1.00  9.18    A   N
ATOM   539 CA  ALA A 69     26.405  62.415  46.244  1.00 10.89    A   C
ATOM   540 CB  ALA A 69     25.129  61.581  46.263  1.00  9.29    A   C
ATOM   541 C   ALA A 69     26.218  63.631  45.358  1.00 10.34    A   C
ATOM   542 O   ALA A 69     26.341  63.546  44.139  1.00 11.20    A   O
ATOM   543 N   CYS A 70     25.905  64.760  45.982  1.00 10.65    A   N
ATOM   544 CA  CYS A 70     25.692  66.000  45.253  1.00 11.99    A   C
ATOM   545 CB  CYS A 70     25.026  67.030  46.167  1.00 13.56    A   C
ATOM   546 SG  CYS A 70     24.697  68.605  45.370  1.00 10.79    A   S
ATOM   547 C   CYS A 70     27.004  66.560  44.720  1.00 11.25    A   C
ATOM   548 O   CYS A 70     27.981  66.708  45.463  1.00  9.23    A   O
ATOM   549 N   ASN A 71     27.030  66.867  43.425  1.00 10.81    A   N
ATOM   550 CA  ASN A 71     28.228  67.424  42.807  1.00  9.85    A   C
ATOM   551 CB  ASN A 71     28.120  67.369  41.285  1.00  7.25    A   C
ATOM   552 CG  ASN A 71     28.026  65.959  40.768  1.00  9.24    A   C
ATOM   553 OD1 ASN A 71     26.998  65.298  40.919  1.00  8.82    A   O
ATOM   554 ND2 ASN A 71     29.107  65.478  40.165  1.00  9.13    A   N
ATOM   555 C   ASN A 71     28.434  68.866  43.246  1.00 12.09    A   C
ATOM   556 O   ASN A 71     29.565  69.321  43.432  1.00  9.50    A   O
ATOM   557 N   THR A 72     27.337  69.593  43.399  1.00 10.94    A   N
ATOM   558 CA  THR A 72     27.436  70.975  43.834  1.00 10.39    A   C
ATOM   559 CB  THR A 72     26.073  71.676  43.779  1.00  9.07    A   C
ATOM   560 OG1 THR A 72     25.599  71.675  42.429  1.00 10.15    A   O
ATOM   561 CG2 THR A 72     26.200  73.122  44.262  1.00  9.53    A   C
ATOM   562 C   THR A 72     27.974  71.029  45.259  1.00 11.47    A   C
ATOM   563 O   THR A 72     28.882  71.808  45.556  1.00  9.49    A   O
ATOM   564 N   ALA A 73     27.415  70.202  46.144  1.00 13.67    A   N
ATOM   565 CA  ALA A 73     27.871  70.171  47.531  1.00 13.27    A   C
ATOM   566 CB  ALA A 73     26.979  69.251  48.368  1.00 15.12    A   C
ATOM   567 C   ALA A 73     29.318  69.691  47.586  1.00 15.74    A   C
ATOM   568 O   ALA A 73     30.111  70.160  48.412  1.00 15.99    A   O
ATOM   569 N   SER A 74     29.660  68.746  46.714  1.00 13.48    A   N
ATOM   570 CA  SER A 74     31.021  68.226  46.677  1.00 13.55    A   C
ATOM   571 CB  SER A 74     31.133  67.078  45.666  1.00 10.32    A   C
ATOM   572 OG  SER A 74     30.483  65.916  46.148  1.00 14.22    A   O
ATOM   573 C   SER A 74     31.994  69.333  46.297  1.00 15.60    A   C
ATOM   574 O   SER A 74     33.093  69.439  46.845  1.00 14.18    A   O
ATOM   575 N   ALA A 75     31.578  70.169  45.359  1.00 13.93    A   N
ATOM   576 CA  ALA A 75     32.422  71.259  44.899  1.00 15.79    A   C
ATOM   577 CB  ALA A 75     31.899  71.773  43.560  1.00 16.15    A   C
ATOM   578 C   ALA A 75     32.549  72.420  45.886  1.00 17.44    A   C
ATOM   579 O   ALA A 75     33.639  72.967  46.063  1.00 18.83    A   O
ATOM   580 N   LEU A 76     31.453  72.777  46.548  1.00 15.33    A   N
ATOM   581 CA  LEU A 76     31.462  73.920  47.460  1.00 17.71    A   C
ATOM   582 CB  LEU A 76     30.236  74.793  47.189  1.00 16.64    A   C
ATOM   583 CG  LEU A 76     30.154  75.642  45.917  1.00 19.98    A   C
ATOM   584 CD1 LEU A 76     30.338  74.793  44.681  1.00 15.78    A   C
ATOM   585 CD2 LEU A 76     28.801  76.343  45.886  1.00 19.48    A   C
ATOM   586 C   LEU A 76     31.544  73.693  48.967  1.00 18.84    A   C
ATOM   587 O   LEU A 76     32.101  74.531  49.685  1.00 17.49    A   O
ATOM   588 N   ALA A 77     30.996  72.584  49.456  1.00 16.91    A   N
ATOM   589 CA  ALA A 77     30.986  72.338  50.896  1.00 17.45    A   C
ATOM   590 CB  ALA A 77     29.546  72.118  51.363  1.00 15.97    A   C
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Figure 5L

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ATOM   591  C   ALA A  77     31.862  71.206  51.422  1.00 17.05      A   C
ATOM   592  O   ALA A  77     32.092  71.120  52.630  1.00 15.31      A   O
ATOM   593  N   LEU A  78     32.355  70.350  50.533  1.00 17.95      A   N
ATOM   594  CA  LEU A  78     33.173  69.217  50.950  1.00 18.28      A   C
ATOM   595  CB  LEU A  78     33.701  68.456  49.726  1.00 17.49      A   C
ATOM   596  CG  LEU A  78     34.425  67.141  50.053  1.00 18.47      A   C
ATOM   597  CD1 LEU A  78     33.467  66.196  50.771  1.00 13.07      A   C
ATOM   598  CD2 LEU A  78     34.949  66.493  48.772  1.00 15.57      A   C
ATOM   599  C   LEU A  78     34.337  69.572  51.873  1.00 19.44      A   C
ATOM   600  O   LEU A  78     34.478  68.986  52.944  1.00 17.85      A   O
ATOM   601  N   GLU A  79     35.173  70.524  51.472  1.00 20.74      A   N
ATOM   602  CA  GLU A  79     36.310  70.897  52.304  1.00 23.29      A   C
ATOM   603  CB  GLU A  79     37.112  72.023  51.652  1.00 25.50      A   C
ATOM   604  CG  GLU A  79     38.332  72.435  52.464  1.00 32.40      A   C
ATOM   605  CD  GLU A  79     39.248  73.382  51.714  1.00 36.37      A   C
ATOM   606  OE1 GLU A  79     38.811  74.501  51.377  1.00 38.33      A   O
ATOM   607  OE2 GLU A  79     40.411  73.002  51.459  1.00 40.30      A   O
ATOM   608  C   GLU A  79     35.900  71.312  53.716  1.00 22.08      A   C
ATOM   609  O   GLU A  79     36.512  70.888  54.691  1.00 22.83      A   O
ATOM   610  N   GLU A  80     34.862  72.132  53.825  1.00 22.05      A   N
ATOM   611  CA  GLU A  80     34.399  72.591  55.125  1.00 21.68      A   C
ATOM   612  CB  GLU A  80     33.336  73.675  54.957  1.00 26.13      A   C
ATOM   613  CG  GLU A  80     33.081  74.457  56.232  1.00 32.22      A   C
ATOM   614  CD  GLU A  80     34.173  75.479  56.521  1.00 34.38      A   C
ATOM   615  OE1 GLU A  80     35.371  75.145  56.399  1.00 36.64      A   O
ATOM   616  OE2 GLU A  80     33.828  76.623  56.878  1.00 38.94      A   O
ATOM   617  C   GLU A  80     33.823  71.435  55.939  1.00 21.19      A   C
ATOM   618  O   GLU A  80     34.013  71.359  57.152  1.00 20.49      A   O
ATOM   619  N   MET A  81     33.116  70.533  55.269  1.00 18.90      A   N
ATOM   620  CA  MET A  81     32.531  69.389  55.950  1.00 16.84      A   C
ATOM   621  CB  MET A  81     31.639  68.605  54.992  1.00 14.00      A   C
ATOM   622  CG  MET A  81     30.375  69.349  54.615  1.00 15.86      A   C
ATOM   623  SD  MET A  81     29.517  68.583  53.244  1.00 15.74      A   S
ATOM   624  CE  MET A  81     28.866  67.134  54.019  1.00 14.04      A   C
ATOM   625  C   MET A  81     33.618  68.474  56.503  1.00 17.31      A   C
ATOM   626  O   MET A  81     33.539  68.020  57.646  1.00 16.49      A   O
ATOM   627  N   GLN A  82     34.632  68.216  55.684  1.00 18.90      A   N
ATOM   628  CA  GLN A  82     35.739  67.351  56.078  1.00 22.12      A   C
ATOM   629  CB  GLN A  82     36.674  67.125  54.887  1.00 22.92      A   C
ATOM   630  CG  GLN A  82     36.001  66.442  53.706  1.00 21.03      A   C
ATOM   631  CD  GLN A  82     36.961  66.158  52.575  1.00 22.15      A   C
ATOM   632  OE1 GLN A  82     37.725  67.033  52.159  1.00 22.13      A   O
ATOM   633  NE2 GLN A  82     36.924  64.934  52.061  1.00 20.69      A   N
ATOM   634  C   GLN A  82     36.516  67.956  57.237  1.00 24.53      A   C
ATOM   635  O   GLN A  82     37.051  67.239  58.086  1.00 23.68      A   O
ATOM   636  N   LYS A  83     36.565  69.282  57.271  1.00 26.24      A   N
ATOM   637  CA  LYS A  83     37.282  69.993  58.317  1.00 30.03      A   C
ATOM   638  CB  LYS A  83     37.178  71.505  58.092  1.00 30.40      A   C
ATOM   639  CG  LYS A  83     38.023  72.336  59.041  1.00 34.26      A   C
ATOM   640  CD  LYS A  83     37.873  73.829  58.756  1.00 38.51      A   C
ATOM   641  CE  LYS A  83     38.287  74.175  57.329  1.00 42.25      A   C
ATOM   642  NZ  LYS A  83     38.067  75.619  57.005  1.00 43.57      A   N
ATOM   643  C   LYS A  83     36.764  69.650  59.708  1.00 30.42      A   C
ATOM   644  O   LYS A  83     37.551  69.395  60.616  1.00 31.77      A   O
ATOM   645  N   TYR A  84     35.445  69.624  59.870  1.00 30.72      A   N
ATOM   646  CA  TYR A  84     34.850  69.341  61.173  1.00 34.49      A   C
ATOM   647  CB  TYR A  84     33.702  70.322  61.441  1.00 38.58      A   C
ATOM   648  CG  TYR A  84     34.109  71.781  61.386  1.00 43.85      A   C
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Figure 5M

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ATOM   649 CD1 TYR A  84      34.172  72.465  60.169  1.00 45.26      A   C
ATOM   650 CE1 TYR A  84      34.575  73.803  60.111  1.00 46.74      A   C
ATOM   651 CD2 TYR A  84      34.460  72.472  62.549  1.00 45.80      A   C
ATOM   652 CE2 TYR A  84      34.865  73.808  62.501  1.00 47.25      A   C
ATOM   653 CZ  TYR A  84      34.920  74.467  61.281  1.00 47.45      A   C
ATOM   654 OH  TYR A  84      35.321  75.784  61.233  1.00 47.13      A   O
ATOM   655 C   TYR A  84      34.349  67.911  61.401  1.00 33.43      A   C
ATOM   656 O   TYR A  84      33.973  67.555  62.520  1.00 34.46      A   O
ATOM   657 N   SER A  85      34.348  67.088  60.361  1.00 30.46      A   N
ATOM   658 CA  SER A  85      33.865  65.721  60.507  1.00 27.21      A   C
ATOM   659 CB  SER A  85      33.384  65.192  59.160  1.00 26.99      A   C
ATOM   660 OG  SER A  85      33.003  63.836  59.279  1.00 27.59      A   O
ATOM   661 C   SER A  85      34.883  64.745  61.088  1.00 25.50      A   C
ATOM   662 O   SER A  85      36.059  64.778  60.730  1.00 24.71      A   O
ATOM   663 N   LYS A  86      34.415  63.875  61.981  1.00 23.68      A   N
ATOM   664 CA  LYS A  86      35.265  62.868  62.609  1.00 23.93      A   C
ATOM   665 CB  LYS A  86      34.741  62.509  64.005  1.00 26.65      A   C
ATOM   666 CG  LYS A  86      34.774  63.644  65.028  1.00 31.69      A   C
ATOM   667 CD  LYS A  86      36.190  63.990  65.491  1.00 34.31      A   C
ATOM   668 CE  LYS A  86      37.015  64.657  64.401  1.00 35.72      A   C
ATOM   669 NZ  LYS A  86      38.359  65.087  64.902  1.00 41.28      A   N
ATOM   670 C   LYS A  86      35.308  61.607  61.752  1.00 22.61      A   C
ATOM   671 O   LYS A  86      36.192  60.765  61.914  1.00 23.21      A   O
ATOM   672 N   ILE A  87      34.337  61.462  60.857  1.00 19.67      A   N
ATOM   673 CA  ILE A  87      34.305  60.302  59.975  1.00 18.68      A   C
ATOM   674 CB  ILE A  87      32.896  59.681  59.888  1.00 18.75      A   C
ATOM   675 CG2 ILE A  87      32.510  59.090  61.233  1.00 18.89      A   C
ATOM   676 CG1 ILE A  87      31.887  60.742  59.433  1.00 21.06      A   C
ATOM   677 CD1 ILE A  87      30.508  60.187  59.086  1.00 18.90      A   C
ATOM   678 C   ILE A  87      34.720  60.751  58.585  1.00 16.98      A   C
ATOM   679 O   ILE A  87      34.614  61.932  58.248  1.00 16.62      A   O
ATOM   680 N   PRO A  88      35.219  59.822  57.761  1.00 17.72      A   N
ATOM   681 CD  PRO A  88      35.548  58.403  57.992  1.00 17.09      A   C
ATOM   682 CA  PRO A  88      35.616  60.247  56.418  1.00 17.99      A   C
ATOM   683 CB  PRO A  88      36.319  59.011  55.857  1.00 19.59      A   C
ATOM   684 CG  PRO A  88      35.648  57.872  56.587  1.00 18.28      A   C
ATOM   685 C   PRO A  88      34.411  60.672  55.577  1.00 19.00      A   C
ATOM   686 O   PRO A  88      33.318  60.125  55.711  1.00 17.80      A   O
ATOM   687 N   ILE A  89      34.622  61.668  54.726  1.00 19.35      A   N
ATOM   688 CA  ILE A  89      33.577  62.163  53.843  1.00 18.35      A   C
ATOM   689 CB  ILE A  89      33.171  63.613  54.196  1.00 18.03      A   C
ATOM   690 CG2 ILE A  89      32.157  64.136  53.185  1.00 16.99      A   C
ATOM   691 CG1 ILE A  89      32.562  63.641  55.598  1.00 18.30      A   C
ATOM   692 CD1 ILE A  89      32.020  64.990  56.011  1.00 26.25      A   C
ATOM   693 C   ILE A  89      34.134  62.108  52.429  1.00 17.01      A   C
ATOM   694 O   ILE A  89      35.206  62.646  52.144  1.00 18.36      A   O
ATOM   695 N   VAL A  90      33.406  61.435  51.551  1.00 15.45      A   N
ATOM   696 CA  VAL A  90      33.829  61.270  50.173  1.00 14.79      A   C
ATOM   697 CB  VAL A  90      33.899  59.779  49.806  1.00 14.33      A   C
ATOM   698 CG1 VAL A  90      34.409  59.605  48.389  1.00 12.10      A   C
ATOM   699 CG2 VAL A  90      34.804  59.055  50.796  1.00 15.51      A   C
ATOM   700 C   VAL A  90      32.858  61.957  49.234  1.00 14.94      A   C
ATOM   701 O   VAL A  90      31.658  61.702  49.283  1.00 15.20      A   O
ATOM   702 N   GLY A  91      33.391  62.830  48.387  1.00 13.93      A   N
ATOM   703 CA  GLY A  91      32.570  63.540  47.427  1.00 14.67      A   C
ATOM   704 C   GLY A  91      32.606  62.829  46.087  1.00 15.17      A   C
ATOM   705 O   GLY A  91      33.262  61.794  45.937  1.00 15.39      A   O
ATOM   706 N   VAL A  92      31.921  63.391  45.101  1.00 13.28      A   N
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Figure 5N

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ATOM   707 CA  VAL A 92     31.871  62.777  43.782  1.00 15.09    A   C
ATOM   708 CB  VAL A 92     30.434  62.762  43.243  1.00 14.78    A   C
ATOM   709 CG1 VAL A 92     29.629  61.703  43.977  1.00 14.03    A   C
ATOM   710 CG2 VAL A 92     29.793  64.135  43.412  1.00 10.70    A   C
ATOM   711 C   VAL A 92     32.770  63.405  42.730  1.00 14.63    A   C
ATOM   712 O   VAL A 92     32.739  63.006  41.567  1.00 17.71    A   O
ATOM   713 N   ILE A 93     33.578  64.378  43.128  1.00 15.55    A   N
ATOM   714 CA  ILE A 93     34.468  65.025  42.176  1.00 16.08    A   C
ATOM   715 CB  ILE A 93     34.684  66.497  42.561  1.00 16.56    A   C
ATOM   716 CG2 ILE A 93     35.653  67.169  41.589  1.00 11.15    A   C
ATOM   717 CG1 ILE A 93     33.329  67.210  42.555  1.00 17.56    A   C
ATOM   718 CD1 ILE A 93     33.385  68.627  43.056  1.00 24.35    A   C
ATOM   719 C   ILE A 93     35.812  64.304  42.032  1.00 15.47    A   C
ATOM   720 O   ILE A 93     36.180  63.904  40.926  1.00 14.93    A   O
ATOM   721 N   GLU A 94     36.536  64.118  43.132  1.00 16.92    A   N
ATOM   722 CA  GLU A 94     37.831  63.446  43.052  1.00 16.92    A   C
ATOM   723 CB  GLU A 94     38.471  63.305  44.434  1.00 20.92    A   C
ATOM   724 CG  GLU A 94     39.894  62.754  44.361  1.00 26.29    A   C
ATOM   725 CD  GLU A 94     40.576  62.678  45.713  1.00 32.62    A   C
ATOM   726 OE1 GLU A 94     40.310  61.723  46.474  1.00 35.02    A   O
ATOM   727 OE2 GLU A 94     41.377  63.588  46.019  1.00 37.91    A   O
ATOM   728 C   GLU A 94     37.745  62.067  42.399  1.00 16.23    A   C
ATOM   729 O   GLU A 94     38.594  61.710  41.578  1.00 12.72    A   O
ATOM   730 N   PRO A 95     36.728  61.263  42.765  1.00 14.67    A   N
ATOM   731 CD  PRO A 95     35.728  61.426  43.835  1.00 11.50    A   C
ATOM   732 CA  PRO A 95     36.612  59.933  42.154  1.00 13.49    A   C
ATOM   733 CB  PRO A 95     35.324  59.385  42.766  1.00 10.50    A   C
ATOM   734 CG  PRO A 95     35.340  59.990  44.132  1.00 13.67    A   C
ATOM   735 C   PRO A 95     36.552  59.995  40.628  1.00 13.36    A   C
ATOM   736 O   PRO A 95     37.111  59.144  39.942  1.00 13.11    A   O
ATOM   737 N   SER A 96     35.868  61.001  40.097  1.00 13.15    A   N
ATOM   738 CA  SER A 96     35.769  61.145  38.652  1.00 13.88    A   C
ATOM   739 CB  SER A 96     34.712  62.190  38.287  1.00 13.27    A   C
ATOM   740 OG  SER A 96     33.415  61.695  38.569  1.00 13.98    A   O
ATOM   741 C   SER A 96     37.121  61.532  38.062  1.00 16.13    A   C
ATOM   742 O   SER A 96     37.482  61.069  36.978  1.00 16.25    A   O
ATOM   743 N   ILE A 97     37.862  62.381  38.774  1.00 16.51    A   N
ATOM   744 CA  ILE A 97     39.181  62.807  38.318  1.00 16.84    A   C
ATOM   745 CB  ILE A 97     39.836  63.786  39.325  1.00 20.72    A   C
ATOM   746 CG2 ILE A 97     41.243  64.165  38.860  1.00 19.14    A   C
ATOM   747 CG1 ILE A 97     38.968  65.039  39.477  1.00 21.89    A   C
ATOM   748 CD1 ILE A 97     38.774  65.827  38.192  1.00 22.65    A   C
ATOM   749 C   ILE A 97     40.070  61.572  38.178  1.00 17.43    A   C
ATOM   750 O   ILE A 97     40.762  61.399  37.171  1.00 16.68    A   O
ATOM   751 N   LEU A 98     40.043  60.716  39.193  1.00 15.65    A   N
ATOM   752 CA  LEU A 98     40.840  59.498  39.182  1.00 18.16    A   C
ATOM   753 CB  LEU A 98     40.749  58.809  40.547  1.00 16.07    A   C
ATOM   754 CG  LEU A 98     41.359  59.641  41.682  1.00 15.84    A   C
ATOM   755 CD1 LEU A 98     41.069  58.980  43.020  1.00 13.47    A   C
ATOM   756 CD2 LEU A 98     42.866  59.788  41.466  1.00 19.12    A   C
ATOM   757 C   LEU A 98     40.374  58.563  38.063  1.00 17.77    A   C
ATOM   758 O   LEU A 98     41.199  57.934  37.389  1.00 16.62    A   O
ATOM   759 N   ALA A 99     39.058  58.485  37.859  1.00 16.23    A   N
ATOM   760 CA  ALA A 99     38.490  57.643  36.807  1.00 18.22    A   C
ATOM   761 CB  ALA A 99     36.962  57.767  36.788  1.00 20.22    A   C
ATOM   762 C   ALA A 99     39.065  58.077  35.462  1.00 17.90    A   C
ATOM   763 O   ALA A 99     39.496  57.246  34.658  1.00 17.01    A   O
ATOM   764 N   ILE A 100    39.067  59.386  35.226  1.00 15.73    A   N
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Figure 5O

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ATOM   765  CA  ILE A 100      39.601  59.939  33.987  1.00 17.26      A   C
ATOM   766  CB  ILE A 100      39.378  61.461  33.932  1.00 12.99      A   C
ATOM   767  CG2 ILE A 100      40.158  62.065  32.772  1.00 16.82      A   C
ATOM   768  CG1 ILE A 100      37.880  61.752  33.795  1.00 15.82      A   C
ATOM   769  CD1 ILE A 100      37.516  63.216  33.925  1.00 14.23      A   C
ATOM   770  C   ILE A 100     41.099  59.640  33.878  1.00 19.31      A   C
ATOM   771  O   ILE A 100     41.594  59.260  32.815  1.00 19.06      A   O
ATOM   772  N   LYS A 101     41.812  59.802  34.986  1.00 19.58      A   N
ATOM   773  CA  LYS A 101      43.246  59.543  35.019  1.00 22.07      A   C
ATOM   774  CB  LYS A 101      43.771  59.741  36.440  1.00 23.70      A   C
ATOM   775  CG  LYS A 101      45.273  59.581  36.595  1.00 28.63      A   C
ATOM   776  CD  LYS A 101      45.671  59.665  38.062  1.00 33.56      A   C
ATOM   777  CE  LYS A 101      47.180  59.570  38.245  1.00 36.39      A   C
ATOM   778  NZ  LYS A 101      47.894  60.739  37.649  1.00 38.26      A   N
ATOM   779  C   LYS A 101     43.538  58.117  34.551  1.00 23.93      A   C
ATOM   780  O   LYS A 101     44.472  57.882  33.780  1.00 23.77      A   O
ATOM   781  N   ARG A 102     42.723  57.174  35.010  1.00 23.37      A   N
ATOM   782  CA  ARG A 102      42.899  55.775  34.655  1.00 25.65      A   C
ATOM   783  CB  ARG A 102      42.096  54.870  35.593  1.00 25.41      A   C
ATOM   784  CG  ARG A 102      42.656  54.749  37.000  1.00 28.61      A   C
ATOM   785  CD  ARG A 102      41.926  53.657  37.782  1.00 31.73      A   C
ATOM   786  NE  ARG A 102      40.486  53.903  37.858  1.00 35.18      A   N
ATOM   787  CZ  ARG A 102      39.903  54.713  38.736  1.00 34.42      A   C
ATOM   788  NH1 ARG A 102      38.586  54.876  38.718  1.00 29.69      A   N
ATOM   789  NH2 ARG A 102      40.637  55.344  39.644  1.00 34.01      A   N
ATOM   790  C   ARG A 102     42.522  55.437  33.222  1.00 26.39      A   C
ATOM   791  O   ARG A 102     43.180  54.611  32.594  1.00 26.86      A   O
ATOM   792  N   GLN A 103     41.473  56.061  32.694  1.00 26.77      A   N
ATOM   793  CA  GLN A 103      41.067  55.733  31.331  1.00 27.82      A   C
ATOM   794  CB  GLN A 103      39.585  55.335  31.306  1.00 28.07      A   C
ATOM   795  CG  GLN A 103      38.661  56.210  32.116  1.00 31.66      A   C
ATOM   796  CD  GLN A 103      37.378  55.489  32.504  1.00 32.01      A   C
ATOM   797  OE1 GLN A 103      36.672  54.951  31.651  1.00 32.82      A   O
ATOM   798  NE2 GLN A 103      37.071  55.479  33.797  1.00 31.78      A   N
ATOM   799  C   GLN A 103     41.363  56.739  30.223  1.00 26.37      A   C
ATOM   800  O   GLN A 103     41.024  56.494  29.066  1.00 26.19      A   O
ATOM   801  N   VAL A 104     42.003  57.856  30.559  1.00 25.47      A   N
ATOM   802  CA  VAL A 104      42.342  58.855  29.550  1.00 24.55      A   C
ATOM   803  CB  VAL A 104      41.542  60.154  29.756  1.00 23.42      A   C
ATOM   804  CG1 VAL A 104      41.998  61.208  28.755  1.00 24.85      A   C
ATOM   805  CG2 VAL A 104      40.055  59.876  29.582  1.00 19.58      A   C
ATOM   806  C   VAL A 104     43.838  59.174  29.578  1.00 26.78      A   C
ATOM   807  O   VAL A 104     44.287  60.043  30.324  1.00 25.34      A   O
ATOM   808  N   GLU A 105     44.601  58.460  28.755  1.00 27.15      A   N
ATOM   809  CA  GLU A 105      46.045  58.641  28.679  1.00 28.29      A   C
ATOM   810  CB  GLU A 105      46.680  57.457  27.947  1.00 33.28      A   C
ATOM   811  CG  GLU A 105      46.743  56.183  28.771  1.00 42.55      A   C
ATOM   812  CD  GLU A 105      47.669  56.315  29.969  1.00 46.07      A   C
ATOM   813  OE1 GLU A 105      47.467  57.242  30.784  1.00 48.67      A   O
ATOM   814  OE2 GLU A 105      48.600  55.491  30.095  1.00 49.87      A   O
ATOM   815  C   GLU A 105     46.461  59.930  27.995  1.00 27.62      A   C
ATOM   816  O   GLU A 105     47.395  60.600  28.437  1.00 27.02      A   O
ATOM   817  N   ASP A 106     45.769  60.273  26.914  1.00 26.11      A   N
ATOM   818  CA  ASP A 106      46.079  61.485  26.164  1.00 25.35      A   C
ATOM   819  CB  ASP A 106      45.271  61.526  24.867  1.00 24.40      A   C
ATOM   820  CG  ASP A 106      45.714  62.641  23.932  1.00 25.06      A   C
ATOM   821  OD1 ASP A 106      46.302  63.640  24.404  1.00 25.51      A   O
ATOM   822  OD2 ASP A 106      45.458  62.522  22.718  1.00 25.51      A   O
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Figure 5P

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ATOM   823  C   ASP A 106     45.759  62.722  26.991  1.00 24.65      A   C
ATOM   824  O   ASP A 106     44.593  63.086  27.142  1.00 24.49      A   O
ATOM   825  N   LYS A 107     46.791  63.372  27.519  1.00 25.06      A   N
ATOM   826  CA  LYS A 107     46.593  64.570  28.327  1.00 24.62      A   C
ATOM   827  CB  LYS A 107     47.919  65.024  28.954  1.00 26.00      A   C
ATOM   828  CG  LYS A 107     48.506  64.047  29.972  1.00 28.40      A   C
ATOM   829  CD  LYS A 107     47.527  63.770  31.107  1.00 26.24      A   C
ATOM   830  CE  LYS A 107     48.086  62.757  32.090  1.00 30.72      A   C
ATOM   831  NZ  LYS A 107     47.086  62.398  33.133  1.00 34.82      A   N
ATOM   832  C   LYS A 107     46.000  65.708  27.503  1.00 24.04      A   C
ATOM   833  O   LYS A 107     45.538  66.706  28.054  1.00 25.01      A   O
ATOM   834  N   ASN A 108     46.014  65.555  26.182  1.00 24.07      A   N
ATOM   835  CA  ASN A 108     45.473  66.572  25.286  1.00 23.49      A   C
ATOM   836  CB  ASN A 108     46.390  66.750  24.073  1.00 23.91      A   C
ATOM   837  CG  ASN A 108     47.596  67.601  24.385  1.00 26.66      A   C
ATOM   838  OD1 ASN A 108     47.464  68.780  24.716  1.00 28.22      A   O
ATOM   839  ND2 ASN A 108     48.780  67.011  24.293  1.00 26.45      A   N
ATOM   840  C   ASN A 108     44.059  66.255  24.818  1.00 21.66      A   C
ATOM   841  O   ASN A 108     43.487  66.983  24.009  1.00 22.58      A   O
ATOM   842  N   ALA A 109     43.494  65.164  25.321  1.00 21.45      A   N
ATOM   843  CA  ALA A 109     42.137  64.793  24.946  1.00 20.49      A   C
ATOM   844  CB  ALA A 109     41.755  63.468  25.599  1.00 21.55      A   C
ATOM   845  C   ALA A 109     41.187  65.902  25.402  1.00 18.98      A   C
ATOM   846  O   ALA A 109     41.237  66.346  26.546  1.00 18.14      A   O
ATOM   847  N   PRO A 110     40.315  66.375  24.505  1.00 19.61      A   N
ATOM   848  CD  PRO A 110     40.090  65.997  23.100  1.00 20.78      A   C
ATOM   849  CA  PRO A 110     39.397  67.436  24.919  1.00 18.53      A   C
ATOM   850  CB  PRO A 110     38.762  67.872  23.606  1.00 18.56      A   C
ATOM   851  CG  PRO A 110     38.726  66.596  22.825  1.00 22.18      A   C
ATOM   852  C   PRO A 110     38.380  66.924  25.928  1.00 17.90      A   C
ATOM   853  O   PRO A 110     37.623  65.996  25.650  1.00 18.78      A   O
ATOM   854  N   ILE A 111     38.384  67.526  27.109  1.00 16.88      A   N
ATOM   855  CA  ILE A 111     37.461  67.137  28.165  1.00 16.87      A   C
ATOM   856  CB  ILE A 111     38.197  66.905  29.503  1.00 17.13      A   C
ATOM   857  CG2 ILE A 111     37.195  66.560  30.592  1.00 18.00      A   C
ATOM   858  CG1 ILE A 111     39.225  65.780  29.352  1.00 16.90      A   C
ATOM   859  CD1 ILE A 111     40.127  65.612  30.574  1.00 20.07      A   C
ATOM   860  C   ILE A 111     36.438  68.246  28.360  1.00 14.74      A   C
ATOM   861  O   ILE A 111     36.792  69.422  28.422  1.00 18.10      A   O
ATOM   862  N   LEU A 112     35.170  67.861  28.450  1.00 15.95      A   N
ATOM   863  CA  LEU A 112     34.086  68.814  28.646  1.00 15.98      A   C
ATOM   864  CB  LEU A 112     33.081  68.715  27.498  1.00 13.81      A   C
ATOM   865  CG  LEU A 112     31.755  69.460  27.703  1.00 17.30      A   C
ATOM   866  CD1 LEU A 112     32.000  70.958  27.834  1.00 12.50      A   C
ATOM   867  CD2 LEU A 112     30.832  69.165  26.524  1.00 17.57      A   C
ATOM   868  C   LEU A 112     33.379  68.527  29.966  1.00 15.50      A   C
ATOM   869  O   LEU A 112     32.823  67.445  30.158  1.00 14.25      A   O
ATOM   870  N   VAL A 113     33.394  69.507  30.864  1.00 15.54      A   N
ATOM   871  CA  VAL A 113     32.767  69.361  32.173  1.00 15.01      A   C
ATOM   872  CB  VAL A 113     33.614  70.035  33.278  1.00 16.33      A   C
ATOM   873  CG1 VAL A 113     33.011  69.752  34.653  1.00 12.34      A   C
ATOM   874  CG2 VAL A 113     35.053  69.538  33.208  1.00 15.51      A   C
ATOM   875  C   VAL A 113     31.390  70.006  32.178  1.00 15.47      A   C
ATOM   876  O   VAL A 113     31.257  71.197  31.901  1.00 15.67      A   O
ATOM   877  N   LEU A 114     30.370  69.215  32.494  1.00 14.67      A   N
ATOM   878  CA  LEU A 114     29.000  69.717  32.554  1.00 13.42      A   C
ATOM   879  CB  LEU A 114     28.074  68.836  31.716  1.00 13.87      A   C
ATOM   880  CG  LEU A 114     28.440  68.622  30.247  1.00 15.67      A   C
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Figure 5Q

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ATOM   881  CD1 LEU A 114     27.349  67.775  29.595  1.00 14.66    A   C
ATOM   882  CD2 LEU A 114     28.583  69.965  29.528  1.00 16.47    A   C
ATOM   883  C   LEU A 114     28.536  69.684  34.006  1.00 12.89    A   C
ATOM   884  O   LEU A 114     28.772  68.706  34.718  1.00 12.06    A   O
ATOM   885  N   GLY A 115     27.873  70.745  34.451  1.00 13.97    A   N
ATOM   886  CA  GLY A 115     27.403  70.763  35.822  1.00 12.19    A   C
ATOM   887  C   GLY A 115     26.528  71.961  36.088  1.00 13.28    A   C
ATOM   888  O   GLY A 115     26.171  72.696  35.160  1.00 14.73    A   O
ATOM   889  N   THR A 116     26.167  72.153  37.351  1.00 11.11    A   N
ATOM   890  CA  THR A 116     25.348  73.297  37.725  1.00 13.32    A   C
ATOM   891  CB  THR A 116     24.866  73.197  39.170  1.00 11.37    A   C
ATOM   892  OG1 THR A 116     26.000  73.180  40.041  1.00 10.70    A   O
ATOM   893  CG2 THR A 116     24.036  71.939  39.367  1.00 10.35    A   C
ATOM   894  C   THR A 116     26.195  74.554  37.614  1.00 14.14    A   C
ATOM   895  O   THR A 116     27.416  74.482  37.431  1.00 14.71    A   O
ATOM   896  N   LYS A 117     25.535  75.701  37.716  1.00 13.99    A   N
ATOM   897  CA  LYS A 117     26.204  76.993  37.657  1.00 14.71    A   C
ATOM   898  CB  LYS A 117     25.147  78.105  37.777  1.00 15.38    A   C
ATOM   899  CG  LYS A 117     25.652  79.472  38.236  1.00 25.83    A   C
ATOM   900  CD  LYS A 117     26.685  80.064  37.296  1.00 33.76    A   C
ATOM   901  CE  LYS A 117     26.103  80.361  35.920  1.00 38.20    A   C
ATOM   902  NZ  LYS A 117     27.105  81.002  35.015  1.00 42.09    A   N
ATOM   903  C   LYS A 117     27.233  77.085  38.787  1.00 12.72    A   C
ATOM   904  O   LYS A 117     28.356  77.549  38.588  1.00 11.82    A   O
ATOM   905  N   ALA A 118     26.854  76.621  39.972  1.00 11.59    A   N
ATOM   906  CA  ALA A 118     27.750  76.671  41.120  1.00 11.90    A   C
ATOM   907  CB  ALA A 118     26.990  76.297  42.382  1.00  8.77    A   C
ATOM   908  C   ALA A 118     28.965  75.758  40.955  1.00 13.39    A   C
ATOM   909  O   ALA A 118     30.099  76.161  41.223  1.00 14.34    A   O
ATOM   910  N   THR A 119     28.721  74.530  40.508  1.00 13.12    A   N
ATOM   911  CA  THR A 119     29.789  73.561  40.316  1.00 12.85    A   C
ATOM   912  CB  THR A 119     29.224  72.205  39.840  1.00 13.42    A   C
ATOM   913  OG1 THR A 119     28.398  71.647  40.869  1.00 11.57    A   O
ATOM   914  CG2 THR A 119     30.353  71.235  39.509  1.00 13.13    A   C
ATOM   915  C   THR A 119     30.808  74.050  39.298  1.00 12.99    A   C
ATOM   916  O   THR A 119     32.016  74.004  39.547  1.00 13.76    A   O
ATOM   917  N   ILE A 120     30.323  74.520  38.154  1.00 11.88    A   N
ATOM   918  CA  ILE A 120     31.213  75.003  37.103  1.00 13.74    A   C
ATOM   919  CB  ILE A 120     30.419  75.310  35.807  1.00 13.41    A   C
ATOM   920  CG2 ILE A 120     31.321  75.980  34.769  1.00 14.31    A   C
ATOM   921  CG1 ILE A 120     29.799  74.012  35.266  1.00 14.49    A   C
ATOM   922  CD1 ILE A 120     30.786  72.862  35.086  1.00 12.48    A   C
ATOM   923  C   ILE A 120     31.977  76.246  37.547  1.00 16.55    A   C
ATOM   924  O   ILE A 120     33.192  76.337  37.372  1.00 18.38    A   O
ATOM   925  N   GLN A 121     31.257  77.200  38.126  1.00 19.17    A   N
ATOM   926  CA  GLN A 121     31.861  78.437  38.601  1.00 20.47    A   C
ATOM   927  CB  GLN A 121     30.790  79.302  39.275  1.00 22.58    A   C
ATOM   928  CG  GLN A 121     31.332  80.406  40.175  1.00 27.23    A   C
ATOM   929  CD  GLN A 121     30.251  81.377  40.627  1.00 30.53    A   C
ATOM   930  OE1 GLN A 121     30.383  82.030  41.664  1.00 32.67    A   O
ATOM   931  NE2 GLN A 121     29.185  81.486  39.842  1.00 28.50    A   N
ATOM   932  C   GLN A 121     33.012  78.170  39.570  1.00 20.02    A   C
ATOM   933  O   GLN A 121     33.979  78.931  39.622  1.00 20.38    A   O
ATOM   934  N   SER A 122     32.905  77.082  40.326  1.00 20.65    A   N
ATOM   935  CA  SER A 122     33.919  76.709  41.311  1.00 19.01    A   C
ATOM   936  CB  SER A 122     33.377  75.609  42.222  1.00 17.57    A   C
ATOM   937  OG  SER A 122     33.446  74.356  41.556  1.00 13.49    A   O
ATOM   938  C   SER A 122     35.220  76.201  40.686  1.00 18.75    A   C
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Figure 5R

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ATOM   939 O   SER A 122    36.270  76.232  41.325  1.00 17.22    A   O
ATOM   940 N   ASN A 123    35.136  75.709  39.454  1.00 18.64    A   N
ATOM   941 CA  ASN A 123    36.292  75.159  38.752  1.00 19.81    A   C
ATOM   942 CB  ASN A 123    37.355  76.237  38.538  1.00 23.62    A   C
ATOM   943 CG  ASN A 123    36.915  77.277  37.537  1.00 27.79    A   C
ATOM   944 OD1 ASN A 123    36.375  76.939  36.483  1.00 25.00    A   O
ATOM   945 ND2 ASN A 123    37.141  78.549  37.855  1.00 30.06    A   N
ATOM   946 C   ASN A 123    36.898  73.967  39.487  1.00 18.35    A   C
ATOM   947 O   ASN A 123    38.057  73.606  39.272  1.00 15.93    A   O
ATOM   948 N   ALA A 124    36.101  73.356  40.356  1.00 16.83    A   N
ATOM   949 CA  ALA A 124    36.550  72.197  41.113  1.00 18.02    A   C
ATOM   950 CB  ALA A 124    35.392  71.613  41.914  1.00 17.02    A   C
ATOM   951 C   ALA A 124    37.109  71.148  40.157  1.00 16.55    A   C
ATOM   952 O   ALA A 124    38.195  70.614  40.376  1.00 17.86    A   O
ATOM   953 N   TYR A 125    36.370  70.858  39.091  1.00 15.55    A   N
ATOM   954 CA  TYR A 125    36.817  69.870  38.121  1.00 15.38    A   C
ATOM   955 CB  TYR A 125    35.699  69.549  37.125  1.00 14.36    A   C
ATOM   956 CG  TYR A 125    34.638  68.609  37.662  1.00 15.54    A   C
ATOM   957 CD1 TYR A 125    33.460  69.096  38.226  1.00 13.69    A   C
ATOM   958 CE1 TYR A 125    32.478  68.230  38.701  1.00 16.51    A   C
ATOM   959 CD2 TYR A 125    34.813  67.224  37.591  1.00 15.03    A   C
ATOM   960 CE2 TYR A 125    33.839  66.349  38.064  1.00 16.83    A   C
ATOM   961 CZ  TYR A 125    32.677  66.857  38.614  1.00 15.95    A   C
ATOM   962 OH  TYR A 125    31.718  65.993  39.065  1.00 16.50    A   O
ATOM   963 C   TYR A 125    38.060  70.323  37.361  1.00 15.65    A   C
ATOM   964 O   TYR A 125    39.050  69.596  37.289  1.00 12.18    A   O
ATOM   965 N   ASP A 126    37.998  71.523  36.796  1.00 15.04    A   N
ATOM   966 CA  ASP A 126    39.110  72.080  36.032  1.00 19.15    A   C
ATOM   967 CB  ASP A 126    38.805  73.530  35.642  1.00 18.87    A   C
ATOM   968 CG  ASP A 126    37.532  73.659  34.831  1.00 21.01    A   C
ATOM   969 OD1 ASP A 126    36.489  73.129  35.271  1.00 22.54    A   O
ATOM   970 OD2 ASP A 126    37.570  74.295  33.756  1.00 22.03    A   O
ATOM   971 C   ASP A 126    40.423  72.028  36.814  1.00 19.26    A   C
ATOM   972 O   ASP A 126    41.432  71.519  36.316  1.00 19.31    A   O
ATOM   973 N   ASN A 127    40.406  72.542  38.040  1.00 18.32    A   N
ATOM   974 CA  ASN A 127    41.613  72.549  38.860  1.00 20.39    A   C
ATOM   975 CB  ASN A 127    41.349  73.226  40.206  1.00 19.27    A   C
ATOM   976 CG  ASN A 127    41.031  74.703  40.067  1.00 23.43    A   C
ATOM   977 OD1 ASN A 127    41.553  75.382  39.185  1.00 25.20    A   O
ATOM   978 ND2 ASN A 127    40.185  75.213  40.955  1.00 22.93    A   N
ATOM   979 C   ASN A 127    42.183  71.155  39.096  1.00 19.69    A   C
ATOM   980 O   ASN A 127    43.381  70.926  38.926  1.00 19.93    A   O
ATOM   981 N   ALA A 128    41.325  70.222  39.488  1.00 17.80    A   N
ATOM   982 CA  ALA A 128    41.767  68.862  39.742  1.00 19.25    A   C
ATOM   983 CB  ALA A 128    40.596  68.016  40.218  1.00 17.14    A   C
ATOM   984 C   ALA A 128    42.383  68.253  38.489  1.00 18.99    A   C
ATOM   985 O   ALA A 128    43.434  67.614  38.553  1.00 21.03    A   O
ATOM   986 N   LEU A 129    41.734  68.456  37.347  1.00 18.35    A   N
ATOM   987 CA  LEU A 129    42.237  67.911  36.088  1.00 18.37    A   C
ATOM   988 CB  LEU A 129    41.229  68.157  34.966  1.00 16.99    A   C
ATOM   989 CG  LEU A 129    39.944  67.331  35.044  1.00 17.37    A   C
ATOM   990 CD1 LEU A 129    38.906  67.908  34.101  1.00 18.55    A   C
ATOM   991 CD2 LEU A 129    40.247  65.878  34.690  1.00 19.31    A   C
ATOM   992 C   LEU A 129    43.586  68.512  35.709  1.00 18.69    A   C
ATOM   993 O   LEU A 129    44.486  67.799  35.264  1.00 16.61    A   O
ATOM   994 N   LYS A 130    43.722  69.823  35.881  1.00 20.51    A   N
ATOM   995 CA  LYS A 130    44.974  70.492  35.559  1.00 25.95    A   C
ATOM   996 CB  LYS A 130    44.869  72.002  35.815  1.00 29.56    A   C
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Figure 5S

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ATOM   997 CG  LYS A 130    44.065  72.756  34.766  1.00 35.38    A   C
ATOM   998 CD  LYS A 130    44.211  74.273  34.910  1.00 40.67    A   C
ATOM   999 CE  LYS A 130    43.491  74.796  36.138  1.00 44.58    A   C
ATOM  1000 NZ  LYS A 130    42.021  74.573  36.036  1.00 48.51    A   N
ATOM  1001 C   LYS A 130    46.084  69.899  36.413  1.00 27.20    A   C
ATOM  1002 O   LYS A 130    47.173  69.607  35.921  1.00 26.83    A   O
ATOM  1003 N   GLN A 131    45.793  69.711  37.695  1.00 27.73    A   N
ATOM  1004 CA  GLN A 131    46.768  69.152  38.615  1.00 30.51    A   C
ATOM  1005 CB  GLN A 131    46.168  69.058  40.017  1.00 34.61    A   C
ATOM  1006 CG  GLN A 131    47.164  68.658  41.086  1.00 44.44    A   C
ATOM  1007 CD  GLN A 131    46.499  68.364  42.414  1.00 49.85    A   C
ATOM  1008 OE1 GLN A 131    45.721  67.415  42.532  1.00 53.57    A   O
ATOM  1009 NE2 GLN A 131    46.797  69.181  43.423  1.00 52.59    A   N
ATOM  1010 C   GLN A 131    47.205  67.769  38.139  1.00 29.59    A   C
ATOM  1011 O   GLN A 131    48.333  67.347  38.389  1.00 27.34    A   O
ATOM  1012 N   GLN A 132    46.311  67.066  37.452  1.00 27.34    A   N
ATOM  1013 CA  GLN A 132    46.634  65.738  36.950  1.00 28.50    A   C
ATOM  1014 CB  GLN A 132    45.382  64.865  36.894  1.00 30.13    A   C
ATOM  1015 CG  GLN A 132    44.863  64.445  38.253  1.00 32.88    A   C
ATOM  1016 CD  GLN A 132    45.924  63.758  39.093  1.00 36.97    A   C
ATOM  1017 OE1 GLN A 132    46.545  62.787  38.659  1.00 36.12    A   O
ATOM  1018 NE2 GLN A 132    46.136  64.262  40.308  1.00 36.40    A   N
ATOM  1019 C   GLN A 132    47.297  65.764  35.579  1.00 26.54    A   C
ATOM  1020 O   GLN A 132    47.465  64.721  34.948  1.00 25.99    A   O
ATOM  1021 N   GLY A 133    47.653  66.958  35.113  1.00 25.65    A   N
ATOM  1022 CA  GLY A 133    48.326  67.079  33.833  1.00 25.61    A   C
ATOM  1023 C   GLY A 133    47.496  67.252  32.575  1.00 26.98    A   C
ATOM  1024 O   GLY A 133    48.061  67.293  31.479  1.00 25.64    A   O
ATOM  1025 N   TYR A 134    46.174  67.353  32.696  1.00 25.10    A   N
ATOM  1026 CA  TYR A 134    45.357  67.526  31.495  1.00 24.59    A   C
ATOM  1027 CB  TYR A 134    43.902  67.120  31.762  1.00 20.44    A   C
ATOM  1028 CG  TYR A 134    43.781  65.626  31.951  1.00 19.78    A   C
ATOM  1029 CD1 TYR A 134    43.870  65.050  33.219  1.00 21.76    A   C
ATOM  1030 CE1 TYR A 134    43.868  63.664  33.380  1.00 19.57    A   C
ATOM  1031 CD2 TYR A 134    43.681  64.774  30.850  1.00 19.08    A   C
ATOM  1032 CE2 TYR A 134    43.682  63.389  31.002  1.00 17.24    A   C
ATOM  1033 CZ  TYR A 134    43.777  62.842  32.265  1.00 18.47    A   C
ATOM  1034 OH  TYR A 134    43.792  61.473  32.413  1.00 19.23    A   O
ATOM  1035 C   TYR A 134    45.461  68.951  30.972  1.00 22.87    A   C
ATOM  1036 O   TYR A 134    45.446  69.908  31.746  1.00 22.48    A   O
ATOM  1037 N   LEU A 135    45.571  69.078  29.650  1.00 22.86    A   N
ATOM  1038 CA  LEU A 135    45.750  70.377  29.008  1.00 24.08    A   C
ATOM  1039 CB  LEU A 135    47.048  70.359  28.192  1.00 24.76    A   C
ATOM  1040 CG  LEU A 135    48.311  69.857  28.906  1.00 25.95    A   C
ATOM  1041 CD1 LEU A 135    49.461  69.790  27.913  1.00 27.98    A   C
ATOM  1042 CD2 LEU A 135    48.658  70.779  30.068  1.00 26.13    A   C
ATOM  1043 C   LEU A 135    44.628  70.873  28.107  1.00 23.53    A   C
ATOM  1044 O   LEU A 135    44.736  71.957  27.539  1.00 24.90    A   O
ATOM  1045 N   ASN A 136    43.556  70.100  27.970  1.00 22.37    A   N
ATOM  1046 CA  ASN A 136    42.450  70.499  27.102  1.00 20.74    A   C
ATOM  1047 CB  ASN A 136    42.411  69.585  25.876  1.00 21.50    A   C
ATOM  1048 CG  ASN A 136    41.613  70.170  24.735  1.00 23.18    A   C
ATOM  1049 OD1 ASN A 136    40.590  70.822  24.945  1.00 25.29    A   O
ATOM  1050 ND2 ASN A 136    42.068  69.923  23.511  1.00 23.17    A   N
ATOM  1051 C   ASN A 136    41.146  70.370  27.887  1.00 20.55    A   C
ATOM  1052 O   ASN A 136    40.430  69.386  27.744  1.00 20.93    A   O
ATOM  1053 N   ILE A 137    40.847  71.371  28.709  1.00 19.65    A   N
ATOM  1054 CA  ILE A 137    39.649  71.347  29.545  1.00 19.51    A   C
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Figure 5T

ATOM 1055 CB ILE A 137 40.021 71.504 31.032 1.00 19.77 A C
ATOM 1056 CG2 ILE A 137 38.792 71.235 31.905 1.00 18.91 A C
ATOM 1057 CG1 ILE A 137 41.165 70.548 31.388 1.00 17.50 A C
ATOM 1058 CD1 ILE A 137 41.841 70.877 32.705 1.00 17.99 A C
ATOM 1059 C ILE A 137 38.650 72.445 29.214 1.00 18.94 A C
ATOM 1060 O ILE A 137 39.008 73.618 29.141 1.00 18.47 A O
ATOM 1061 N SER A 138 37.394 72.054 29.019 1.00 18.59 A N
ATOM 1062 CA SER A 138 36.319 73.000 28.729 1.00 19.77 A C
ATOM 1063 CB SER A 138 35.810 72.829 27.294 1.00 21.73 A C
ATOM 1064 OG SER A 138 36.823 73.104 26.345 1.00 24.47 A O
ATOM 1065 C SER A 138 35.177 72.716 29.698 1.00 19.64 A C
ATOM 1066 O SER A 138 34.971 71.569 30.102 1.00 20.10 A O
ATOM 1067 N HIS A 139 34.443 73.753 30.083 1.00 18.51 A N
ATOM 1068 CA HIS A 139 33.319 73.565 30.993 1.00 18.98 A C
ATOM 1069 CB HIS A 139 33.697 73.982 32.418 1.00 18.17 A C
ATOM 1070 CG HIS A 139 34.220 75.380 32.522 1.00 19.94 A C
ATOM 1071 CD2 HIS A 139 33.634 76.575 32.268 1.00 20.85 A C
ATOM 1072 ND1 HIS A 139 35.506 75.661 32.926 1.00 20.98 A N
ATOM 1073 CE1 HIS A 139 35.692 76.970 32.916 1.00 24.03 A C
ATOM 1074 NE2 HIS A 139 34.572 77.547 32.520 1.00 22.03 A N
ATOM 1075 C HIS A 139 32.082 74.329 30.552 1.00 18.46 A C
ATOM 1076 O HIS A 139 32.181 75.372 29.909 1.00 19.58 A O
ATOM 1077 N LEU A 140 30.918 73.791 30.902 1.00 18.71 A N
ATOM 1078 CA LEU A 140 29.634 74.403 30.573 1.00 19.01 A C
ATOM 1079 CB LEU A 140 29.028 73.775 29.316 1.00 20.85 A C
ATOM 1080 CG LEU A 140 29.476 74.190 27.918 1.00 22.92 A C
ATOM 1081 CD1 LEU A 140 28.667 73.394 26.904 1.00 21.79 A C
ATOM 1082 CD2 LEU A 140 29.255 75.688 27.709 1.00 25.42 A C
ATOM 1083 C LEU A 140 28.632 74.227 31.702 1.00 17.69 A C
ATOM 1084 O LEU A 140 28.422 73.118 32.194 1.00 17.06 A O
ATOM 1085 N ALA A 141 28.008 75.322 32.112 1.00 18.99 A N
ATOM 1086 CA ALA A 141 26.995 75.256 33.153 1.00 18.92 A C
ATOM 1087 CB ALA A 141 26.976 76.553 33.955 1.00 19.92 A C
ATOM 1088 C ALA A 141 25.653 75.046 32.456 1.00 20.05 A C
ATOM 1089 O ALA A 141 25.002 76.007 32.053 1.00 22.92 A O
ATOM 1090 N THR A 142 25.250 73.790 32.299 1.00 17.67 A N
ATOM 1091 CA THR A 142 23.983 73.456 31.650 1.00 15.92 A C
ATOM 1092 CB THR A 142 24.069 72.061 30.991 1.00 15.55 A C
ATOM 1093 OG1 THR A 142 24.474 71.094 31.969 1.00 15.28 A O
ATOM 1094 CG2 THR A 142 25.091 72.069 29.862 1.00 16.16 A C
ATOM 1095 C THR A 142 22.890 73.462 32.725 1.00 16.51 A C
ATOM 1096 O THR A 142 22.195 72.469 32.942 1.00 15.07 A O
ATOM 1097 N SER A 143 22.746 74.608 33.382 1.00 15.40 A N
ATOM 1098 CA SER A 143 21.797 74.779 34.479 1.00 16.69 A C
ATOM 1099 CB SER A 143 21.745 76.254 34.886 1.00 18.40 A C
ATOM 1100 OG SER A 143 20.979 76.419 36.068 1.00 19.14 A O
ATOM 1101 C SER A 143 20.374 74.259 34.266 1.00 16.28 A C
ATOM 1102 O SER A 143 19.838 73.555 35.119 1.00 17.50 A O
ATOM 1103 N LEU A 144 19.766 74.597 33.133 1.00 15.61 A N
ATOM 1104 CA LEU A 144 18.397 74.174 32.850 1.00 16.29 A C
ATOM 1105 CB LEU A 144 17.920 74.855 31.567 1.00 18.23 A C
ATOM 1106 CG LEU A 144 17.915 76.379 31.743 1.00 21.65 A C
ATOM 1107 CD1 LEU A 144 17.543 77.079 30.440 1.00 21.02 A C
ATOM 1108 CD2 LEU A 144 16.931 76.741 32.854 1.00 19.77 A C
ATOM 1109 C LEU A 144 18.171 72.657 32.772 1.00 15.16 A C
ATOM 1110 O LEU A 144 17.036 72.184 32.874 1.00 13.64 A O
ATOM 1111 N PHE A 145 19.238 71.888 32.600 1.00 13.93 A N
ATOM 1112 CA PHE A 145 19.080 70.437 32.545 1.00 11.95 A C

Figure 5U

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ATOM  1113  CB  PHE A 145      20.436  69.742  32.374  1.00 13.43      A   C
ATOM  1114  CG  PHE A 145      21.000  69.808  30.976  1.00 17.43      A   C
ATOM  1115  CD1 PHE A 145      22.248  69.260  30.703  1.00 15.45      A   C
ATOM  1116  CD2 PHE A 145      20.287  70.399  29.933  1.00 17.04      A   C
ATOM  1117  CE1 PHE A 145      22.783  69.295  29.420  1.00 18.35      A   C
ATOM  1118  CE2 PHE A 145      20.815  70.440  28.642  1.00 15.38      A   C
ATOM  1119  CZ  PHE A 145      22.064  69.889  28.385  1.00 16.89      A   C
ATOM  1120  C   PHE A 145      18.436  69.956  33.846  1.00 12.03      A   C
ATOM  1121  O   PHE A 145      17.600  69.064  33.839  1.00 11.95      A   O
ATOM  1122  N   VAL A 146      18.813  70.564  34.965  1.00 12.43      A   N
ATOM  1123  CA  VAL A 146      18.269  70.150  36.255  1.00 11.55      A   C
ATOM  1124  CB  VAL A 146      18.931  70.941  37.420  1.00 11.44      A   C
ATOM  1125  CG1 VAL A 146      18.203  70.669  38.739  1.00 12.27      A   C
ATOM  1126  CG2 VAL A 146      20.389  70.523  37.541  1.00 12.17      A   C
ATOM  1127  C   VAL A 146      16.741  70.243  36.344  1.00 13.17      A   C
ATOM  1128  O   VAL A 146      16.081  69.236  36.566  1.00 13.35      A   O
ATOM  1129  N   PRO A 147      16.157  71.442  36.168  1.00 14.55      A   N
ATOM  1130  CD  PRO A 147      16.725  72.794  36.014  1.00 12.51      A   C
ATOM  1131  CA  PRO A 147      14.693  71.491  36.260  1.00 15.45      A   C
ATOM  1132  CB  PRO A 147      14.386  72.995  36.197  1.00 16.91      A   C
ATOM  1133  CG  PRO A 147      15.556  73.569  35.463  1.00 13.21      A   C
ATOM  1134  C   PRO A 147      13.972  70.682  35.178  1.00 13.90      A   C
ATOM  1135  O   PRO A 147      12.910  70.111  35.433  1.00 15.62      A   O
ATOM  1136  N   LEU A 148      14.549  70.614  33.982  1.00 11.79      A   N
ATOM  1137  CA  LEU A 148      13.929  69.844  32.911  1.00 13.83      A   C
ATOM  1138  CB  LEU A 148      14.748  69.947  31.620  1.00 15.89      A   C
ATOM  1139  CG  LEU A 148      14.193  70.877  30.540  1.00 14.82      A   C
ATOM  1140  CD1 LEU A 148      14.146  72.296  31.057  1.00 18.80      A   C
ATOM  1141  CD2 LEU A 148      15.070  70.792  29.300  1.00 16.16      A   C
ATOM  1142  C   LEU A 148      13.833  68.389  33.336  1.00 13.84      A   C
ATOM  1143  O   LEU A 148      12.786  67.755  33.204  1.00 15.22      A   O
ATOM  1144  N   ILE A 149      14.935  67.872  33.861  1.00 12.81      A   N
ATOM  1145  CA  ILE A 149      14.985  66.493  34.312  1.00 13.21      A   C
ATOM  1146  CB  ILE A 149      16.425  66.111  34.703  1.00 14.51      A   C
ATOM  1147  CG2 ILE A 149      16.444  64.756  35.402  1.00 12.63      A   C
ATOM  1148  CG1 ILE A 149      17.291  66.093  33.434  1.00 15.10      A   C
ATOM  1149  CD1 ILE A 149      18.777  65.893  33.673  1.00 10.57      A   C
ATOM  1150  C   ILE A 149      14.026  66.258  35.470  1.00 14.45      A   C
ATOM  1151  O   ILE A 149      13.425  65.195  35.571  1.00 15.79      A   O
ATOM  1152  N   GLU A 150      13.859  67.256  36.328  1.00 14.06      A   N
ATOM  1153  CA  GLU A 150      12.943  67.121  37.449  1.00 15.01      A   C
ATOM  1154  CB  GLU A 150      13.206  68.228  38.466  1.00 18.77      A   C
ATOM  1155  CG  GLU A 150      14.447  67.930  39.291  1.00 26.06      A   C
ATOM  1156  CD  GLU A 150      14.824  69.044  40.227  1.00 28.16      A   C
ATOM  1157  OE1 GLU A 150      15.731  68.821  41.056  1.00 26.46      A   O
ATOM  1158  OE2 GLU A 150      14.222  70.138  40.128  1.00 31.52      A   O
ATOM  1159  C   GLU A 150      11.481  67.116  37.000  1.00 15.40      A   C
ATOM  1160  O   GLU A 150      10.615  66.617  37.719  1.00 14.17      A   O
ATOM  1161  N   GLU A 151      11.212  67.680  35.822  1.00 13.23      A   N
ATOM  1162  CA  GLU A 151       9.860  67.703  35.265  1.00 15.55      A   C
ATOM  1163  CB  GLU A 151       9.619  68.971  34.442  1.00 16.54      A   C
ATOM  1164  CG  GLU A 151       9.533  70.248  35.267  1.00 20.37      A   C
ATOM  1165  CD  GLU A 151       8.528  70.151  36.401  1.00 23.39      A   C
ATOM  1166  OE1 GLU A 151       7.332  69.901  36.134  1.00 24.54      A   O
ATOM  1167  OE2 GLU A 151       8.937  70.326  37.566  1.00 27.18      A   O
ATOM  1168  C   GLU A 151       9.687  66.487  34.368  1.00 17.22      A   C
ATOM  1169  O   GLU A 151       8.668  66.331  33.687  1.00 16.37      A   O
ATOM  1170  N   SER A 152      10.702  65.632  34.376  1.00 18.04      A   N
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Figure 5V

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ATOM  1171  CA  SER A 152      10.722  64.413  33.578  1.00 18.02      A   C
ATOM  1172  CB  SER A 152       9.559  63.493  33.949  1.00 19.94      A   C
ATOM  1173  OG  SER A 152       9.768  62.207  33.390  1.00 18.81      A   O
ATOM  1174  C   SER A 152      10.699  64.673  32.081  1.00 20.44      A   C
ATOM  1175  O   SER A 152      10.013  63.980  31.323  1.00 22.59      A   O
ATOM  1176  N   ILE A 153      11.443  65.682  31.653  1.00 19.73      A   N
ATOM  1177  CA  ILE A 153      11.541  65.998  30.239  1.00 21.13      A   C
ATOM  1178  CB  ILE A 153      11.541  67.521  30.016  1.00 23.26      A   C
ATOM  1179  CG2 ILE A 153      11.800  67.846  28.546  1.00 22.78      A   C
ATOM  1180  CG1 ILE A 153      10.190  68.086  30.474  1.00 25.17      A   C
ATOM  1181  CD1 ILE A 153      10.005  69.547  30.207  1.00 30.23      A   C
ATOM  1182  C   ILE A 153      12.865  65.372  29.832  1.00 21.67      A   C
ATOM  1183  O   ILE A 153      13.900  66.037  29.784  1.00 20.32      A   O
ATOM  1184  N   LEU A 154      12.811  64.069  29.565  1.00 18.75      A   N
ATOM  1185  CA  LEU A 154      13.986  63.281  29.218  1.00 20.85      A   C
ATOM  1186  CB  LEU A 154      13.939  61.972  30.003  1.00 21.22      A   C
ATOM  1187  CG  LEU A 154      13.540  62.197  31.467  1.00 22.53      A   C
ATOM  1188  CD1 LEU A 154      13.353  60.868  32.182  1.00 21.31      A   C
ATOM  1189  CD2 LEU A 154      14.604  63.040  32.154  1.00 20.71      A   C
ATOM  1190  C   LEU A 154      14.131  62.994  27.726  1.00 21.27      A   C
ATOM  1191  O   LEU A 154      14.969  62.194  27.313  1.00 20.75      A   O
ATOM  1192  N   GLU A 155      13.302  63.649  26.927  1.00 23.77      A   N
ATOM  1193  CA  GLU A 155      13.333  63.499  25.478  1.00 26.10      A   C
ATOM  1194  CB  GLU A 155      12.948  62.069  25.074  1.00 30.66      A   C
ATOM  1195  CG  GLU A 155      11.661  61.554  25.686  1.00 38.37      A   C
ATOM  1196  CD  GLU A 155      10.445  61.898  24.860  1.00 42.76      A   C
ATOM  1197  OE1 GLU A 155       9.322  61.571  25.299  1.00 48.12      A   O
ATOM  1198  OE2 GLU A 155      10.609  62.488  23.771  1.00 46.52      A   O
ATOM  1199  C   GLU A 155      12.366  64.517  24.893  1.00 24.72      A   C
ATOM  1200  O   GLU A 155      11.759  65.288  25.633  1.00 23.59      A   O
ATOM  1201  N   GLY A 156      12.236  64.538  23.573  1.00 23.02      A   N
ATOM  1202  CA  GLY A 156      11.333  65.492  22.958  1.00 21.08      A   C
ATOM  1203  C   GLY A 156      12.047  66.742  22.485  1.00 22.30      A   C
ATOM  1204  O   GLY A 156      13.243  66.925  22.728  1.00 21.15      A   O
ATOM  1205  N   GLU A 157      11.299  67.612  21.817  1.00 20.99      A   N
ATOM  1206  CA  GLU A 157      11.847  68.844  21.268  1.00 22.12      A   C
ATOM  1207  CB  GLU A 157      10.786  69.539  20.412  1.00 25.41      A   C
ATOM  1208  CG  GLU A 157      11.366  70.505  19.398  1.00 32.26      A   C
ATOM  1209  CD  GLU A 157      10.304  71.341  18.720  1.00 37.00      A   C
ATOM  1210  OE1 GLU A 157       9.332  70.758  18.186  1.00 41.42      A   O
ATOM  1211  OE2 GLU A 157      10.443  72.583  18.719  1.00 39.91      A   O
ATOM  1212  C   GLU A 157      12.386  69.835  22.302  1.00 19.65      A   C
ATOM  1213  O   GLU A 157      13.377  70.518  22.053  1.00 18.65      A   O
ATOM  1214  N   LEU A 158      11.734  69.925  23.453  1.00 18.49      A   N
ATOM  1215  CA  LEU A 158      12.172  70.861  24.485  1.00 20.02      A   C
ATOM  1216  CB  LEU A 158      11.174  70.870  25.653  1.00 19.53      A   C
ATOM  1217  CG  LEU A 158      11.410  71.891  26.773  1.00 21.01      A   C
ATOM  1218  CD1 LEU A 158      11.661  73.280  26.191  1.00 20.32      A   C
ATOM  1219  CD2 LEU A 158      10.197  71.910  27.697  1.00 19.63      A   C
ATOM  1220  C   LEU A 158      13.581  70.529  24.976  1.00 17.50      A   C
ATOM  1221  O   LEU A 158      14.424  71.417  25.101  1.00 17.99      A   O
ATOM  1222  N   LEU A 159      13.846  69.253  25.240  1.00 18.72      A   N
ATOM  1223  CA  LEU A 159      15.180  68.856  25.693  1.00 17.84      A   C
ATOM  1224  CB  LEU A 159      15.202  67.377  26.105  1.00 17.62      A   C
ATOM  1225  CG  LEU A 159      16.585  66.818  26.488  1.00 16.01      A   C
ATOM  1226  CD1 LEU A 159      17.125  67.557  27.713  1.00 16.76      A   C
ATOM  1227  CD2 LEU A 159      16.478  65.324  26.775  1.00 16.92      A   C
ATOM  1228  C   LEU A 159      16.185  69.091  24.571  1.00 18.06      A   C
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Figure 5W

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ATOM  1229  O  LEU A 159    17.274  69.629  24.792  1.00 15.90    A   O
ATOM  1230  N  GLU A 160    15.805  68.686  23.363  1.00 17.23    A   N
ATOM  1231  CA  GLU A 160    16.660  68.846  22.199  1.00 19.74    A   C
ATOM  1232  CB  GLU A 160    15.936  68.322  20.951  1.00 22.63    A   C
ATOM  1233  CG  GLU A 160    16.613  68.624  19.612  1.00 25.09    A   C
ATOM  1234  CD  GLU A 160    18.020  68.058  19.496  1.00 28.46    A   C
ATOM  1235  OE1 GLU A 160    18.320  67.041  20.156  1.00 24.99    A   O
ATOM  1236  OE2 GLU A 160    18.824  68.626  18.725  1.00 29.33    A   O
ATOM  1237  C  GLU A 160    17.025  70.316  22.023  1.00 17.75    A   C
ATOM  1238  O  GLU A 160    18.188  70.655  21.795  1.00 17.75    A   O
ATOM  1239  N  THR A 161    16.031  71.188  22.140  1.00 15.91    A   N
ATOM  1240  CA  THR A 161    16.274  72.615  21.984  1.00 17.08    A   C
ATOM  1241  CB  THR A 161    14.955  73.402  21.946  1.00 19.03    A   C
ATOM  1242  OG1 THR A 161    14.165  72.943  20.841  1.00 18.83    A   O
ATOM  1243  CG2 THR A 161    15.225  74.888  21.770  1.00 18.63    A   C
ATOM  1244  C  THR A 161    17.159  73.154  23.104  1.00 16.80    A   C
ATOM  1245  O  THR A 161    17.998  74.029  22.875  1.00 16.81    A   O
ATOM  1246  N  CYS A 162    16.977  72.623  24.309  1.00 15.47    A   N
ATOM  1247  CA  CYS A 162    17.772  73.054  25.451  1.00 16.48    A   C
ATOM  1248  CB  CYS A 162    17.217  72.456  26.748  1.00 17.44    A   C
ATOM  1249  SG  CYS A 162    17.994  73.125  28.246  1.00 17.16    A   S
ATOM  1250  C  CYS A 162    19.226  72.624  25.264  1.00 16.12    A   C
ATOM  1251  O  CYS A 162    20.148  73.390  25.547  1.00 15.64    A   O
ATOM  1252  N  MET A 163    19.433  71.395  24.797  1.00 16.12    A   N
ATOM  1253  CA  MET A 163    20.792  70.913  24.578  1.00 16.90    A   C
ATOM  1254  CB  MET A 163    20.796  69.446  24.152  1.00 17.54    A   C
ATOM  1255  CG  MET A 163    20.259  68.491  25.198  1.00 18.15    A   C
ATOM  1256  SD  MET A 163    20.679  66.775  24.864  1.00 18.78    A   S
ATOM  1257  CE  MET A 163    19.539  66.408  23.514  1.00 18.51    A   C
ATOM  1258  C  MET A 163    21.427  71.760  23.483  1.00 16.80    A   C
ATOM  1259  O  MET A 163    22.601  72.109  23.554  1.00 17.90    A   O
ATOM  1260  N  HIS A 164    20.637  72.083  22.467  1.00 17.35    A   N
ATOM  1261  CA  HIS A 164    21.119  72.893  21.359  1.00 18.77    A   C
ATOM  1262  CB  HIS A 164    20.009  73.065  20.317  1.00 21.03    A   C
ATOM  1263  CG  HIS A 164    20.451  73.784  19.082  1.00 26.61    A   C
ATOM  1264  CD2 HIS A 164    20.862  73.317  17.879  1.00 27.02    A   C
ATOM  1265  ND1 HIS A 164    20.559  75.156  19.018  1.00 26.82    A   N
ATOM  1266  CE1 HIS A 164    21.020  75.503  17.829  1.00 28.20    A   C
ATOM  1267  NE2 HIS A 164    21.212  74.406  17.119  1.00 26.69    A   N
ATOM  1268  C  HIS A 164    21.573  74.249  21.872  1.00 17.93    A   C
ATOM  1269  O  HIS A 164    22.630  74.758  21.483  1.00 18.32    A   O
ATOM  1270  N  TYR A 165    20.775  74.821  22.765  1.00 16.78    A   N
ATOM  1271  CA  TYR A 165    21.073  76.120  23.352  1.00 17.03    A   C
ATOM  1272  CB  TYR A 165    20.004  76.486  24.383  1.00 16.70    A   C
ATOM  1273  CG  TYR A 165    20.323  77.728  25.186  1.00 14.36    A   C
ATOM  1274  CD1 TYR A 165    20.249  78.998  24.611  1.00 18.03    A   C
ATOM  1275  CE1 TYR A 165    20.567  80.144  25.350  1.00 17.68    A   C
ATOM  1276  CD2 TYR A 165    20.722  77.633  26.518  1.00 15.98    A   C
ATOM  1277  CE2 TYR A 165    21.042  78.767  27.263  1.00 15.67    A   C
ATOM  1278  CZ  TYR A 165    20.964  80.015  26.675  1.00 17.67    A   C
ATOM  1279  OH  TYR A 165    21.296  81.128  27.414  1.00 19.35    A   O
ATOM  1280  C  TYR A 165    22.440  76.144  24.025  1.00 18.18    A   C
ATOM  1281  O  TYR A 165    23.202  77.089  23.848  1.00 18.56    A   O
ATOM  1282  N  TYR A 166    22.745  75.101  24.795  1.00 16.65    A   N
ATOM  1283  CA  TYR A 166    24.016  75.022  25.516  1.00 16.14    A   C
ATOM  1284  CB  TYR A 166    23.879  74.113  26.745  1.00 15.22    A   C
ATOM  1285  CG  TYR A 166    23.063  74.681  27.887  1.00 14.44    A   C
ATOM  1286  CD1 TYR A 166    21.955  73.994  28.380  1.00 13.39    A   C
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Figure 5X

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ATOM  1287 CE1 TYR A 166    21.202  74.506  29.438  1.00 14.31    A   C
ATOM  1288 CD2 TYR A 166    23.403  75.898  28.481  1.00 14.07    A   C
ATOM  1289 CE2 TYR A 166    22.660  76.419  29.537  1.00 13.27    A   C
ATOM  1290 CZ  TYR A 166    21.558  75.717  30.008  1.00 15.59    A   C
ATOM  1291 OH  TYR A 166    20.800  76.228  31.033  1.00 13.70    A   O
ATOM  1292 C   TYR A 166    25.207  74.520  24.710  1.00 16.15    A   C
ATOM  1293 O   TYR A 166    26.320  75.020  24.862  1.00 18.32    A   O
ATOM  1294 N   PHE A 167    24.977  73.532  23.858  1.00 16.40    A   N
ATOM  1295 CA  PHE A 167    26.063  72.926  23.099  1.00 19.32    A   C
ATOM  1296 CB  PHE A 167    25.696  71.466  22.811  1.00 18.55    A   C
ATOM  1297 CG  PHE A 167    25.487  70.633  24.056  1.00 17.57    A   C
ATOM  1298 CD1 PHE A 167    24.611  69.551  24.044  1.00 17.73    A   C
ATOM  1299 CD2 PHE A 167    26.179  70.920  25.232  1.00 17.53    A   C
ATOM  1300 CE1 PHE A 167    24.429  68.766  25.186  1.00 17.59    A   C
ATOM  1301 CE2 PHE A 167    26.005  70.140  26.378  1.00 15.09    A   C
ATOM  1302 CZ  PHE A 167    25.130  69.063  26.354  1.00 15.31    A   C
ATOM  1303 C   PHE A 167    26.517  73.613  21.810  1.00 21.91    A   C
ATOM  1304 O   PHE A 167    27.693  73.529  21.444  1.00 18.63    A   O
ATOM  1305 N   THR A 168    25.600  74.293  21.128  1.00 23.53    A   N
ATOM  1306 CA  THR A 168    25.940  74.958  19.871  1.00 25.11    A   C
ATOM  1307 CB  THR A 168    24.757  75.788  19.346  1.00 24.47    A   C
ATOM  1308 OG1 THR A 168    23.646  74.919  19.099  1.00 28.03    A   O
ATOM  1309 CG2 THR A 168    25.133  76.488  18.048  1.00 28.49    A   C
ATOM  1310 C   THR A 168    27.182  75.849  19.920  1.00 24.43    A   C
ATOM  1311 O   THR A 168    27.989  75.836  18.995  1.00 26.62    A   O
ATOM  1312 N   PRO A 169    27.347  76.640  20.992  1.00 25.87    A   N
ATOM  1313 CD  PRO A 169    26.337  76.983  22.009  1.00 23.89    A   C
ATOM  1314 CA  PRO A 169    28.512  77.523  21.113  1.00 28.42    A   C
ATOM  1315 CB  PRO A 169    28.198  78.329  22.372  1.00 25.95    A   C
ATOM  1316 CG  PRO A 169    26.709  78.406  22.351  1.00 26.22    A   C
ATOM  1317 C   PRO A 169    29.868  76.813  21.210  1.00 30.41    A   C
ATOM  1318 O   PRO A 169    30.914  77.440  21.035  1.00 30.45    A   O
ATOM  1319 N   LEU A 170    29.853  75.512  21.487  1.00 32.27    A   N
ATOM  1320 CA  LEU A 170    31.094  74.755  21.611  1.00 34.59    A   C
ATOM  1321 CB  LEU A 170    30.808  73.338  22.098  1.00 33.83    A   C
ATOM  1322 CG  LEU A 170    30.417  73.202  23.568  1.00 32.01    A   C
ATOM  1323 CD1 LEU A 170    30.035  71.760  23.848  1.00 29.69    A   C
ATOM  1324 CD2 LEU A 170    31.579  73.641  24.458  1.00 29.22    A   C
ATOM  1325 C   LEU A 170    31.897  74.677  20.323  1.00 37.74    A   C
ATOM  1326 O   LEU A 170    31.358  74.386  19.254  1.00 39.31    A   O
ATOM  1327 N   GLU A 171    33.197  74.924  20.434  1.00 40.03    A   N
ATOM  1328 CA  GLU A 171    34.076  74.871  19.276  1.00 43.34    A   C
ATOM  1329 CB  GLU A 171    34.750  76.229  19.067  1.00 48.27    A   C
ATOM  1330 CG  GLU A 171    33.759  77.349  18.782  1.00 54.56    A   C
ATOM  1331 CD  GLU A 171    33.072  77.200  17.431  1.00 59.45    A   C
ATOM  1332 OE1 GLU A 171    32.919  76.051  16.953  1.00 60.27    A   O
ATOM  1333 OE2 GLU A 171    32.672  78.237  16.852  1.00 61.77    A   O
ATOM  1334 C   GLU A 171    35.120  73.777  19.447  1.00 42.59    A   C
ATOM  1335 O   GLU A 171    36.239  73.888  18.951  1.00 43.77    A   O
ATOM  1336 N   ILE A 172    34.741  72.717  20.155  1.00 40.35    A   N
ATOM  1337 CA  ILE A 172    35.636  71.589  20.391  1.00 38.22    A   C
ATOM  1338 CB  ILE A 172    36.155  71.569  21.842  1.00 37.75    A   C
ATOM  1339 CG2 ILE A 172    36.806  72.901  22.184  1.00 34.13    A   C
ATOM  1340 CG1 ILE A 172    34.997  71.276  22.797  1.00 36.28    A   C
ATOM  1341 CD1 ILE A 172    35.430  70.993  24.225  1.00 40.90    A   C
ATOM  1342 C   ILE A 172    34.911  70.272  20.145  1.00 36.42    A   C
ATOM  1343 O   ILE A 172    33.688  70.200  20.222  1.00 39.20    A   O
ATOM  1344 N   LEU A 173    35.674  69.231  19.838  1.00 34.80    A   N
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Figure 5Y

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ATOM  1345 CA  LEU A 173     35.104  67.910  19.612  1.00 32.15      A   C
ATOM  1346 CB  LEU A 173     35.718  67.265  18.363  1.00 33.04      A   C
ATOM  1347 CG  LEU A 173     35.480  67.998  17.037  1.00 34.61      A   C
ATOM  1348 CD1 LEU A 173     36.221  67.290  15.910  1.00 33.74      A   C
ATOM  1349 CD2 LEU A 173     33.979  68.056  16.747  1.00 34.77      A   C
ATOM  1350 C   LEU A 173     35.454  67.102  20.855  1.00 29.45      A   C
ATOM  1351 O   LEU A 173     36.481  66.424  20.896  1.00 27.62      A   O
ATOM  1352 N   PRO A 174     34.598  67.167  21.891  1.00 27.18      A   N
ATOM  1353 CD  PRO A 174     33.272  67.811  21.931  1.00 26.43      A   C
ATOM  1354 CA  PRO A 174     34.858  66.432  23.132  1.00 24.33      A   C
ATOM  1355 CB  PRO A 174     33.646  66.772  24.003  1.00 25.04      A   C
ATOM  1356 CG  PRO A 174     32.560  67.015  22.997  1.00 27.39      A   C
ATOM  1357 C   PRO A 174     35.067  64.934  22.991  1.00 21.39      A   C
ATOM  1358 O   PRO A 174     34.335  64.250  22.277  1.00 22.17      A   O
ATOM  1359 N   GLU A 175     36.088  64.438  23.679  1.00 19.42      A   N
ATOM  1360 CA  GLU A 175     36.405  63.021  23.683  1.00 19.85      A   C
ATOM  1361 CB  GLU A 175     37.905  62.821  23.465  1.00 21.90      A   C
ATOM  1362 CG  GLU A 175     38.320  62.869  21.999  1.00 27.70      A   C
ATOM  1363 CD  GLU A 175     39.823  62.943  21.802  1.00 27.64      A   C
ATOM  1364 OE1 GLU A 175     40.565  62.242  22.523  1.00 28.19      A   O
ATOM  1365 OE2 GLU A 175     40.260  63.701  20.913  1.00 30.42      A   O
ATOM  1366 C   GLU A 175     35.983  62.473  25.044  1.00 19.80      A   C
ATOM  1367 O   GLU A 175     35.855  61.263  25.239  1.00 19.75      A   O
ATOM  1368 N   VAL A 176     35.762  63.383  25.986  1.00 18.80      A   N
ATOM  1369 CA  VAL A 176     35.349  63.006  27.330  1.00 17.58      A   C
ATOM  1370 CB  VAL A 176     36.550  62.981  28.313  1.00 16.92      A   C
ATOM  1371 CG1 VAL A 176     36.091  62.488  29.676  1.00 15.99      A   C
ATOM  1372 CG2 VAL A 176     37.661  62.087  27.772  1.00 16.67      A   C
ATOM  1373 C   VAL A 176     34.330  64.014  27.840  1.00 16.96      A   C
ATOM  1374 O   VAL A 176     34.533  65.224  27.746  1.00 17.95      A   O
ATOM  1375 N   ILE A 177     33.222  63.509  28.362  1.00 17.35      A   N
ATOM  1376 CA  ILE A 177     32.184  64.373  28.902  1.00 15.36      A   C
ATOM  1377 CB  ILE A 177     30.873  64.272  28.100  1.00 15.94      A   C
ATOM  1378 CG2 ILE A 177     29.805  65.149  28.759  1.00 14.07      A   C
ATOM  1379 CG1 ILE A 177     31.113  64.699  26.647  1.00 17.19      A   C
ATOM  1380 CD1 ILE A 177     29.880  64.597  25.748  1.00 18.12      A   C
ATOM  1381 C   ILE A 177     31.896  63.970  30.334  1.00 14.25      A   C
ATOM  1382 O   ILE A 177     31.499  62.833  30.609  1.00 15.75      A   O
ATOM  1383 N   ILE A 178     32.108  64.900  31.253  1.00 14.90      A   N
ATOM  1384 CA  ILE A 178     31.841  64.618  32.647  1.00 12.36      A   C
ATOM  1385 CB  ILE A 178     32.770  65.419  33.573  1.00 14.08      A   C
ATOM  1386 CG2 ILE A 178     32.465  65.085  35.026  1.00 10.97      A   C
ATOM  1387 CG1 ILE A 178     34.229  65.095  33.248  1.00 13.91      A   C
ATOM  1388 CD1 ILE A 178     35.235  65.846  34.106  1.00 13.08      A   C
ATOM  1389 C   ILE A 178     30.396  64.988  32.950  1.00 12.88      A   C
ATOM  1390 O   ILE A 178     29.949  66.103  32.671  1.00 13.50      A   O
ATOM  1391 N   LEU A 179     29.659  64.038  33.506  1.00 12.90      A   N
ATOM  1392 CA  LEU A 179     28.270  64.288  33.867  1.00 14.35      A   C
ATOM  1393 CB  LEU A 179     27.465  62.992  33.717  1.00 14.31      A   C
ATOM  1394 CG  LEU A 179     27.542  62.418  32.298  1.00 15.12      A   C
ATOM  1395 CD1 LEU A 179     26.919  61.033  32.251  1.00 20.10      A   C
ATOM  1396 CD2 LEU A 179     26.844  63.361  31.336  1.00 20.25      A   C
ATOM  1397 C   LEU A 179     28.320  64.760  35.319  1.00 13.67      A   C
ATOM  1398 O   LEU A 179     27.829  64.085  36.224  1.00 15.54      A   O
ATOM  1399 N   GLY A 180     28.930  65.931  35.512  1.00 11.65      A   N
ATOM  1400 CA  GLY A 180     29.117  66.517  36.834  1.00 12.90      A   C
ATOM  1401 C   GLY A 180     27.910  67.040  37.593  1.00 10.74      A   C
ATOM  1402 O   GLY A 180     27.955  68.116  38.191  1.00 12.43      A   O
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Figure 5Z

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ATOM  1403 N   CYS A 181    26.835 66.267 37.589 1.00 11.19    A   N
ATOM  1404 CA  CYS A 181    25.608 66.640 38.287 1.00 12.85    A   C
ATOM  1405 CB  CYS A 181    24.832 67.662 37.455 1.00 10.63    A   C
ATOM  1406 SG  CYS A 181    23.232 68.156 38.139 1.00 12.80    A   S
ATOM  1407 C   CYS A 181    24.769 65.379 38.482 1.00 10.40    A   C
ATOM  1408 O   CYS A 181    24.655 64.567 37.565 1.00 12.33    A   O
ATOM  1409 N   THR A 182    24.195 65.218 39.673 1.00 11.84    A   N
ATOM  1410 CA  THR A 182    23.374 64.050 39.993 1.00 10.35    A   C
ATOM  1411 CB  THR A 182    22.661 64.207 41.363 1.00 10.67    A   C
ATOM  1412 OG1 THR A 182    21.912 65.435 41.381 1.00 8.58     A   O
ATOM  1413 CG2 THR A 182    23.672 64.197 42.500 1.00 7.64     A   C
ATOM  1414 C   THR A 182    22.283 63.760 38.966 1.00 11.06    A   C
ATOM  1415 O   THR A 182    21.936 62.610 38.733 1.00 10.76    A   O
ATOM  1416 N   HIS A 183    21.739 64.810 38.364 1.00 9.82     A   N
ATOM  1417 CA  HIS A 183    20.649 64.666 37.400 1.00 12.23    A   C
ATOM  1418 CB  HIS A 183    19.884 65.990 37.276 1.00 10.20    A   C
ATOM  1419 CG  HIS A 183    19.136 66.386 38.510 1.00 10.97    A   C
ATOM  1420 CD2 HIS A 183    17.905 66.930 38.668 1.00 7.50     A   C
ATOM  1421 ND1 HIS A 183    19.677 66.290 39.774 1.00 11.77    A   N
ATOM  1422 CE1 HIS A 183    18.812 66.758 40.658 1.00 10.61    A   C
ATOM  1423 NE2 HIS A 183    17.729 67.154 40.012 1.00 10.59    A   N
ATOM  1424 C   HIS A 183    21.020 64.221 35.990 1.00 10.73    A   C
ATOM  1425 O   HIS A 183    20.228 63.569 35.323 1.00 12.38    A   O
ATOM  1426 N   PHE A 184    22.221 64.570 35.545 1.00 12.86    A   N
ATOM  1427 CA  PHE A 184    22.645 64.280 34.180 1.00 12.13    A   C
ATOM  1428 CB  PHE A 184    23.988 64.976 33.925 1.00 11.91    A   C
ATOM  1429 CG  PHE A 184    23.927 66.488 34.096 1.00 11.77    A   C
ATOM  1430 CD1 PHE A 184    25.057 67.276 33.896 1.00 13.67    A   C
ATOM  1431 CD2 PHE A 184    22.739 67.116 34.482 1.00 9.45     A   C
ATOM  1432 CE1 PHE A 184    25.009 68.666 34.081 1.00 11.33    A   C
ATOM  1433 CE2 PHE A 184    22.681 68.502 34.670 1.00 12.83    A   C
ATOM  1434 CZ  PHE A 184    23.819 69.278 34.469 1.00 9.95     A   C
ATOM  1435 C   PHE A 184    22.655 62.833 33.670 1.00 12.53    A   C
ATOM  1436 O   PHE A 184    22.429 62.596 32.481 1.00 14.09    A   O
ATOM  1437 N   PRO A 185    22.902 61.847 34.545 1.00 13.81    A   N
ATOM  1438 CD  PRO A 185    23.442 61.881 35.918 1.00 14.48    A   C
ATOM  1439 CA  PRO A 185    22.893 60.475 34.026 1.00 13.96    A   C
ATOM  1440 CB  PRO A 185    23.165 59.640 35.275 1.00 14.58    A   C
ATOM  1441 CG  PRO A 185    24.112 60.522 36.032 1.00 12.13    A   C
ATOM  1442 C   PRO A 185    21.554 60.121 33.367 1.00 15.04    A   C
ATOM  1443 O   PRO A 185    21.492 59.261 32.489 1.00 13.75    A   O
ATOM  1444 N   LEU A 186    20.485 60.790 33.791 1.00 13.98    A   N
ATOM  1445 CA  LEU A 186    19.156 60.525 33.243 1.00 13.19    A   C
ATOM  1446 CB  LEU A 186    18.080 61.193 34.108 1.00 13.71    A   C
ATOM  1447 CG  LEU A 186    17.634 60.379 35.334 1.00 15.55    A   C
ATOM  1448 CD1 LEU A 186    18.802 60.174 36.288 1.00 18.92    A   C
ATOM  1449 CD2 LEU A 186    16.493 61.099 36.027 1.00 14.26    A   C
ATOM  1450 C   LEU A 186    18.982 60.931 31.778 1.00 14.41    A   C
ATOM  1451 O   LEU A 186    18.010 60.533 31.137 1.00 14.59    A   O
ATOM  1452 N   ILE A 187    19.905 61.734 31.255 1.00 14.30    A   N
ATOM  1453 CA  ILE A 187    19.854 62.140 29.849 1.00 14.33    A   C
ATOM  1454 CB  ILE A 187    19.485 63.633 29.667 1.00 13.17    A   C
ATOM  1455 CG2 ILE A 187    18.052 63.871 30.096 1.00 11.03    A   C
ATOM  1456 CG1 ILE A 187    20.446 64.523 30.453 1.00 12.17    A   C
ATOM  1457 CD1 ILE A 187    20.256 66.011 30.170 1.00 14.07    A   C
ATOM  1458 C   ILE A 187    21.197 61.890 29.168 1.00 14.64    A   C
ATOM  1459 O   ILE A 187    21.487 62.447 28.108 1.00 13.68    A   O
ATOM  1460 N   ALA A 188    22.008 61.035 29.781 1.00 15.37    A   N
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Figure 5AA

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ATOM  1461  CA  ALA A 188      23.322  60.707  29.243  1.00 16.86      A   C
ATOM  1462  CB  ALA A 188      23.965  59.607  30.075  1.00 15.17      A   C
ATOM  1463  C   ALA A 188      23.244  60.280  27.776  1.00 17.17      A   C
ATOM  1464  O   ALA A 188      23.979  60.797  26.938  1.00 15.74      A   O
ATOM  1465  N   GLN A 189      22.353  59.340  27.470  1.00 17.32      A   N
ATOM  1466  CA  GLN A 189      22.203  58.857  26.101  1.00 18.82      A   C
ATOM  1467  CB  GLN A 189      21.162  57.741  26.050  1.00 23.61      A   C
ATOM  1468  CG  GLN A 189      21.199  56.919  24.774  1.00 30.80      A   C
ATOM  1469  CD  GLN A 189      22.592  56.391  24.458  1.00 36.03      A   C
ATOM  1470  OE1 GLN A 189      23.321  55.942  25.347  1.00 36.39      A   O
ATOM  1471  NE2 GLN A 189      22.965  56.435  23.184  1.00 38.93      A   N
ATOM  1472  C   GLN A 189      21.794  59.995  25.169  1.00 17.49      A   C
ATOM  1473  O   GLN A 189      22.280  60.092  24.041  1.00 17.22      A   O
ATOM  1474  N   LYS A 190      20.894  60.851  25.639  1.00 17.64      A   N
ATOM  1475  CA  LYS A 190      20.449  61.986  24.841  1.00 16.93      A   C
ATOM  1476  CB  LYS A 190      19.338  62.750  25.565  1.00 17.51      A   C
ATOM  1477  CG  LYS A 190      17.998  62.038  25.578  1.00 21.98      A   C
ATOM  1478  CD  LYS A 190      17.462  61.852  24.166  1.00 25.56      A   C
ATOM  1479  CE  LYS A 190      16.064  61.256  24.188  1.00 30.02      A   C
ATOM  1480  NZ  LYS A 190      15.428  61.242  22.839  1.00 32.59      A   N
ATOM  1481  C   LYS A 190      21.624  62.919  24.572  1.00 17.12      A   C
ATOM  1482  O   LYS A 190      21.755  63.468  23.481  1.00 19.51      A   O
ATOM  1483  N   ILE A 191      22.483  63.097  25.570  1.00 15.92      A   N
ATOM  1484  CA  ILE A 191      23.643  63.963  25.413  1.00 15.53      A   C
ATOM  1485  CB  ILE A 191      24.348  64.194  26.769  1.00 16.74      A   C
ATOM  1486  CG2 ILE A 191      25.698  64.877  26.558  1.00 17.54      A   C
ATOM  1487  CG1 ILE A 191      23.447  65.048  27.668  1.00 16.67      A   C
ATOM  1488  CD1 ILE A 191      24.051  65.372  29.014  1.00 17.95      A   C
ATOM  1489  C   ILE A 191      24.615  63.350  24.413  1.00 17.26      A   C
ATOM  1490  O   ILE A 191      25.099  64.027  23.508  1.00 16.51      A   O
ATOM  1491  N   GLU A 192      24.892  62.062  24.566  1.00 17.44      A   N
ATOM  1492  CA  GLU A 192      25.792  61.387  23.643  1.00 18.42      A   C
ATOM  1493  CB  GLU A 192      25.937  59.909  24.007  1.00 20.11      A   C
ATOM  1494  CG  GLU A 192      26.885  59.159  23.085  1.00 26.76      A   C
ATOM  1495  CD  GLU A 192      26.872  57.665  23.322  1.00 32.66      A   C
ATOM  1496  OE1 GLU A 192      25.884  57.005  22.936  1.00 37.07      A   O
ATOM  1497  OE2 GLU A 192      27.846  57.152  23.906  1.00 37.14      A   O
ATOM  1498  C   GLU A 192      25.209  61.499  22.241  1.00 17.46      A   C
ATOM  1499  O   GLU A 192      25.912  61.804  21.283  1.00 15.49      A   O
ATOM  1500  N   GLY A 193      23.910  61.249  22.136  1.00 19.60      A   N
ATOM  1501  CA  GLY A 193      23.247  61.319  20.851  1.00 18.22      A   C
ATOM  1502  C   GLY A 193      23.344  62.683  20.199  1.00 20.98      A   C
ATOM  1503  O   GLY A 193      23.518  62.781  18.983  1.00 19.02      A   O
ATOM  1504  N   TYR A 194      23.230  63.742  20.997  1.00 19.99      A   N
ATOM  1505  CA  TYR A 194      23.302  65.087  20.450  1.00 19.30      A   C
ATOM  1506  CB  TYR A 194      23.081  66.136  21.545  1.00 21.79      A   C
ATOM  1507  CG  TYR A 194      23.038  67.544  20.997  1.00 22.73      A   C
ATOM  1508  CD1 TYR A 194      21.822  68.170  20.713  1.00 25.33      A   C
ATOM  1509  CE1 TYR A 194      21.784  69.442  20.133  1.00 26.15      A   C
ATOM  1510  CD2 TYR A 194      24.216  68.226  20.692  1.00 24.23      A   C
ATOM  1511  CE2 TYR A 194      24.190  69.493  20.109  1.00 23.26      A   C
ATOM  1512  CZ  TYR A 194      22.973  70.092  19.830  1.00 25.26      A   C
ATOM  1513  OH  TYR A 194      22.941  71.327  19.222  1.00 28.86      A   O
ATOM  1514  C   TYR A 194      24.660  65.313  19.788  1.00 20.71      A   C
ATOM  1515  O   TYR A 194      24.738  65.782  18.653  1.00 18.94      A   O
ATOM  1516  N   PHE A 195      25.732  64.980  20.496  1.00 19.26      A   N
ATOM  1517  CA  PHE A 195      27.062  65.169  19.942  1.00 21.38      A   C
ATOM  1518  CB  PHE A 195      28.126  64.952  21.020  1.00 20.73      A   C
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Figure 5BB

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ATOM  1519  CG  PHE A 195      28.251  66.103  21.971  1.00 20.61      A   C
ATOM  1520  CD1 PHE A 195      27.488  66.158  23.131  1.00 19.23      A   C
ATOM  1521  CD2 PHE A 195      29.097  67.165  21.673  1.00 21.43      A   C
ATOM  1522  CE1 PHE A 195      27.565  67.263  23.986  1.00 20.28      A   C
ATOM  1523  CE2 PHE A 195      29.183  68.273  22.515  1.00 18.52      A   C
ATOM  1524  CZ  PHE A 195      28.416  68.323  23.673  1.00 19.62      A   C
ATOM  1525  C   PHE A 195      27.352  64.290  18.730  1.00 21.31      A   C
ATOM  1526  O   PHE A 195      28.045  64.713  17.806  1.00 21.45      A   O
ATOM  1527  N   MET A 196      26.822  63.072  18.720  1.00 22.22      A   N
ATOM  1528  CA  MET A 196      27.059  62.190  17.584  1.00 24.31      A   C
ATOM  1529  CB  MET A 196      26.655  60.749  17.915  1.00 25.67      A   C
ATOM  1530  CG  MET A 196      27.528  60.084  18.971  1.00 26.49      A   C
ATOM  1531  SD  MET A 196      29.295  60.205  18.575  1.00 30.70      A   S
ATOM  1532  CE  MET A 196      29.481  58.865  17.401  1.00 31.02      A   C
ATOM  1533  C   MET A 196      26.293  62.667  16.354  1.00 25.42      A   C
ATOM  1534  O   MET A 196      26.734  62.451  15.227  1.00 23.73      A   O
ATOM  1535  N   GLY A 197      25.157  63.328  16.571  1.00 25.90      A   N
ATOM  1536  CA  GLY A 197      24.361  63.805  15.451  1.00 26.44      A   C
ATOM  1537  C   GLY A 197      24.566  65.258  15.054  1.00 29.06      A   C
ATOM  1538  O   GLY A 197      24.129  65.681  13.981  1.00 30.51      A   O
ATOM  1539  N   HIS A 198      25.233  66.030  15.903  1.00 27.75      A   N
ATOM  1540  CA  HIS A 198      25.456  67.441  15.612  1.00 28.55      A   C
ATOM  1541  CB  HIS A 198      24.824  68.293  16.705  1.00 28.88      A   C
ATOM  1542  CG  HIS A 198      23.330  68.234  16.718  1.00 26.12      A   C
ATOM  1543  CD2 HIS A 198      22.470  67.535  17.495  1.00 26.28      A   C
ATOM  1544  ND1 HIS A 198      22.553  68.943  15.828  1.00 27.58      A   N
ATOM  1545  CE1 HIS A 198      21.277  68.687  16.060  1.00 27.01      A   C
ATOM  1546  NE2 HIS A 198      21.200  67.835  17.066  1.00 26.83      A   N
ATOM  1547  C   HIS A 198      26.923  67.792  15.457  1.00 30.79      A   C
ATOM  1548  O   HIS A 198      27.270  68.941  15.180  1.00 32.29      A   O
ATOM  1549  N   PHE A 199      27.785  66.800  15.644  1.00 30.80      A   N
ATOM  1550  CA  PHE A 199      29.220  66.999  15.498  1.00 33.66      A   C
ATOM  1551  CB  PHE A 199      29.906  67.052  16.866  1.00 35.46      A   C
ATOM  1552  CG  PHE A 199      29.565  68.275  17.676  1.00 39.04      A   C
ATOM  1553  CD1 PHE A 199      28.281  68.463  18.182  1.00 39.24      A   C
ATOM  1554  CD2 PHE A 199      30.537  69.237  17.945  1.00 40.88      A   C
ATOM  1555  CE1 PHE A 199      27.968  69.591  18.944  1.00 40.57      A   C
ATOM  1556  CE2 PHE A 199      30.236  70.370  18.707  1.00 42.99      A   C
ATOM  1557  CZ  PHE A 199      28.948  70.547  19.207  1.00 40.25      A   C
ATOM  1558  C   PHE A 199      29.790  65.855  14.673  1.00 32.87      A   C
ATOM  1559  O   PHE A 199      29.170  64.798  14.547  1.00 32.00      A   O
ATOM  1560  N   ALA A 200      30.972  66.064  14.108  1.00 34.09      A   N
ATOM  1561  CA  ALA A 200      31.605  65.040  13.288  1.00 34.34      A   C
ATOM  1562  CB  ALA A 200      32.381  65.690  12.154  1.00 35.22      A   C
ATOM  1563  C   ALA A 200      32.532  64.168  14.119  1.00 34.93      A   C
ATOM  1564  O   ALA A 200      33.704  63.996  13.782  1.00 35.08      A   O
ATOM  1565  N   LEU A 201      32.012  63.618  15.209  1.00 34.85      A   N
ATOM  1566  CA  LEU A 201      32.821  62.765  16.067  1.00 34.78      A   C
ATOM  1567  CB  LEU A 201      32.210  62.690  17.472  1.00 35.79      A   C
ATOM  1568  CG  LEU A 201      32.120  64.015  18.231  1.00 35.31      A   C
ATOM  1569  CD1 LEU A 201      31.513  63.760  19.603  1.00 35.13      A   C
ATOM  1570  CD2 LEU A 201      33.498  64.641  18.365  1.00 35.35      A   C
ATOM  1571  C   LEU A 201      32.906  61.366  15.462  1.00 34.07      A   C
ATOM  1572  O   LEU A 201      31.887  60.773  15.104  1.00 35.38      A   O
ATOM  1573  N   PRO A 202      34.128  60.817  15.344  1.00 33.66      A   N
ATOM  1574  CD  PRO A 202      35.409  61.457  15.698  1.00 32.39      A   C
ATOM  1575  CA  PRO A 202      34.353  59.475  14.779  1.00 32.85      A   C
ATOM  1576  CB  PRO A 202      35.872  59.404  14.655  1.00 33.65      A   C
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Figure 5CC

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ATOM  1577  CG  PRO A 202      36.343  60.272  15.793  1.00 34.48      A   C
ATOM  1578  C   PRO A 202      33.790  58.355  15.649  1.00 33.17      A   C
ATOM  1579  O   PRO A 202      33.402  57.297  15.151  1.00 30.49      A   O
ATOM  1580  N   THR A 203      33.773  58.599  16.956  1.00 31.52      A   N
ATOM  1581  CA  THR A 203      33.248  57.634  17.919  1.00 31.65      A   C
ATOM  1582  CB  THR A 203      34.338  56.676  18.426  1.00 32.68      A   C
ATOM  1583  OG1 THR A 203      35.425  57.424  18.979  1.00 35.29      A   O
ATOM  1584  CG2 THR A 203      34.828  55.781  17.302  1.00 37.32      A   C
ATOM  1585  C   THR A 203      32.688  58.386  19.117  1.00 30.86      A   C
ATOM  1586  O   THR A 203      33.168  59.451  19.461  1.00 27.18      A   O
ATOM  1587  N   PRO A 204      31.671  57.817  19.775  1.00 29.89      A   N
ATOM  1588  CD  PRO A 204      31.126  56.473  19.492  1.00 29.77      A   C
ATOM  1589  CA  PRO A 204      31.061  58.463  20.945  1.00 28.24      A   C
ATOM  1590  CB  PRO A 204      30.047  57.449  21.462  1.00 29.94      A   C
ATOM  1591  CG  PRO A 204      30.111  56.276  20.568  1.00 30.77      A   C
ATOM  1592  C   PRO A 204      32.096  58.803  22.007  1.00 25.79      A   C
ATOM  1593  O   PRO A 204      33.032  58.041  22.269  1.00 25.89      A   O
ATOM  1594  N   PRO A 205      31.961  59.981  22.626  1.00 23.44      A   N
ATOM  1595  CD  PRO A 205      30.990  61.063  22.358  1.00 24.13      A   C
ATOM  1596  CA  PRO A 205      32.915  60.378  23.670  1.00 22.08      A   C
ATOM  1597  CB  PRO A 205      32.600  61.852  23.873  1.00 24.52      A   C
ATOM  1598  CG  PRO A 205      31.125  61.932  23.587  1.00 24.69      A   C
ATOM  1599  C   PRO A 205      32.705  59.546  24.927  1.00 19.36      A   C
ATOM  1600  O   PRO A 205      31.637  58.961  25.125  1.00 18.49      A   O
ATOM  1601  N   LEU A 206      33.722  59.492  25.776  1.00 18.43      A   N
ATOM  1602  CA  LEU A 206      33.626  58.762  27.037  1.00 18.50      A   C
ATOM  1603  CB  LEU A 206      35.018  58.513  27.619  1.00 20.51      A   C
ATOM  1604  CG  LEU A 206      35.095  57.847  28.996  1.00 22.39      A   C
ATOM  1605  CD1 LEU A 206      34.491  56.439  28.946  1.00 22.36      A   C
ATOM  1606  CD2 LEU A 206      36.552  57.791  29.435  1.00 24.60      A   C
ATOM  1607  C   LEU A 206      32.822  59.615  28.017  1.00 18.04      A   C
ATOM  1608  O   LEU A 206      33.163  60.770  28.253  1.00 16.95      A   O
ATOM  1609  N   LEU A 207      31.746  59.049  28.554  1.00 16.00      A   N
ATOM  1610  CA  LEU A 207      30.909  59.748  29.521  1.00 17.26      A   C
ATOM  1611  CB  LEU A 207      29.433  59.412  29.304  1.00 18.06      A   C
ATOM  1612  CG  LEU A 207      28.664  60.071  28.158  1.00 24.42      A   C
ATOM  1613  CD1 LEU A 207      29.448  59.984  26.863  1.00 25.51      A   C
ATOM  1614  CD2 LEU A 207      27.310  59.373  28.012  1.00 24.48      A   C
ATOM  1615  C   LEU A 207      31.318  59.314  30.922  1.00 16.98      A   C
ATOM  1616  O   LEU A 207      31.388  58.120  31.215  1.00 18.46      A   O
ATOM  1617  N   ILE A 208      31.592  60.276  31.792  1.00 13.50      A   N
ATOM  1618  CA  ILE A 208      31.983  59.940  33.150  1.00 14.98      A   C
ATOM  1619  CB  ILE A 208      33.112  60.864  33.659  1.00 16.20      A   C
ATOM  1620  CG2 ILE A 208      33.468  60.509  35.101  1.00 16.97      A   C
ATOM  1621  CG1 ILE A 208      34.345  60.722  32.763  1.00 16.39      A   C
ATOM  1622  CD1 ILE A 208      34.984  59.333  32.784  1.00 17.91      A   C
ATOM  1623  C   ILE A 208      30.771  60.069  34.057  1.00 15.79      A   C
ATOM  1624  O   ILE A 208      30.193  61.150  34.194  1.00 15.47      A   O
ATOM  1625  N   HIS A 209      30.390  58.951  34.669  1.00 15.02      A   N
ATOM  1626  CA  HIS A 209      29.238  58.895  35.567  1.00 14.90      A   C
ATOM  1627  CB  HIS A 209      28.502  57.569  35.333  1.00 17.49      A   C
ATOM  1628  CG  HIS A 209      27.271  57.387  36.169  1.00 19.71      A   C
ATOM  1629  CD2 HIS A 209      27.116  57.192  37.500  1.00 20.19      A   C
ATOM  1630  ND1 HIS A 209      26.004  57.336  35.625  1.00 21.72      A   N
ATOM  1631  CE1 HIS A 209      25.123  57.114  36.584  1.00 17.63      A   C
ATOM  1632  NE2 HIS A 209      25.772  57.023  37.732  1.00 22.48      A   N
ATOM  1633  C   HIS A 209      29.744  59.006  37.011  1.00 13.24      A   C
ATOM  1634  O   HIS A 209      30.546  58.191  37.458  1.00 13.01      A   O
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Figure 5DD

ATOM 1635 N SER A 210 29.275 60.018 37.734 1.00 12.05 A N
ATOM 1636 CA SER A 210 29.709 60.238 39.109 1.00 11.23 A C
ATOM 1637 CB SER A 210 28.977 61.442 39.701 1.00 11.83 A C
ATOM 1638 OG SER A 210 29.140 62.587 38.881 1.00 12.14 A O
ATOM 1639 C SER A 210 29.529 59.031 40.032 1.00 12.17 A C
ATOM 1640 O SER A 210 30.370 58.774 40.890 1.00 11.45 A O
ATOM 1641 N GLY A 211 28.432 58.303 39.861 1.00 13.88 A N
ATOM 1642 CA GLY A 211 28.178 57.142 40.698 1.00 15.08 A C
ATOM 1643 C GLY A 211 29.147 56.004 40.446 1.00 16.38 A C
ATOM 1644 O GLY A 211 29.744 55.461 41.378 1.00 15.04 A O
ATOM 1645 N ASP A 212 29.311 55.630 39.183 1.00 15.98 A N
ATOM 1646 CA ASP A 212 30.231 54.552 38.860 1.00 16.82 A C
ATOM 1647 CB ASP A 212 30.208 54.264 37.365 1.00 19.63 A C
ATOM 1648 CG ASP A 212 28.847 53.798 36.895 1.00 23.61 A C
ATOM 1649 OD1 ASP A 212 28.145 53.131 37.692 1.00 25.34 A O
ATOM 1650 OD2 ASP A 212 28.486 54.086 35.738 1.00 21.50 A O
ATOM 1651 C ASP A 212 31.638 54.917 39.303 1.00 16.04 A C
ATOM 1652 O ASP A 212 32.375 54.073 39.807 1.00 15.40 A O
ATOM 1653 N ALA A 213 31.994 56.185 39.135 1.00 12.67 A N
ATOM 1654 CA ALA A 213 33.317 56.667 39.517 1.00 14.11 A C
ATOM 1655 CB ALA A 213 33.493 58.126 39.076 1.00 11.29 A C
ATOM 1656 C ALA A 213 33.560 56.540 41.022 1.00 12.53 A C
ATOM 1657 O ALA A 213 34.607 56.049 41.452 1.00 13.00 A O
ATOM 1658 N ILE A 214 32.603 56.973 41.834 1.00 13.61 A N
ATOM 1659 CA ILE A 214 32.808 56.875 43.271 1.00 11.94 A C
ATOM 1660 CB ILE A 214 31.748 57.701 44.065 1.00 12.63 A C
ATOM 1661 CG2 ILE A 214 30.367 57.085 43.938 1.00 15.04 A C
ATOM 1662 CG1 ILE A 214 32.174 57.795 45.530 1.00 12.30 A C
ATOM 1663 CD1 ILE A 214 31.429 58.832 46.317 1.00 11.04 A C
ATOM 1664 C ILE A 214 32.855 55.405 43.719 1.00 13.71 A C
ATOM 1665 O ILE A 214 33.595 55.061 44.643 1.00 12.81 A O
ATOM 1666 N VAL A 215 32.096 54.538 43.053 1.00 13.33 A N
ATOM 1667 CA VAL A 215 32.118 53.109 43.387 1.00 13.18 A C
ATOM 1668 CB VAL A 215 31.165 52.293 42.474 1.00 13.68 A C
ATOM 1669 CG1 VAL A 215 31.481 50.792 42.579 1.00 14.80 A C
ATOM 1670 CG2 VAL A 215 29.707 52.537 42.876 1.00 10.93 A C
ATOM 1671 C VAL A 215 33.550 52.599 43.190 1.00 15.07 A C
ATOM 1672 O VAL A 215 34.115 51.933 44.065 1.00 12.73 A O
ATOM 1673 N GLU A 216 34.136 52.924 42.039 1.00 13.86 A N
ATOM 1674 CA GLU A 216 35.503 52.511 41.738 1.00 17.89 A C
ATOM 1675 CB GLU A 216 35.973 53.120 40.414 1.00 21.27 A C
ATOM 1676 CG GLU A 216 35.112 52.807 39.204 1.00 27.92 A C
ATOM 1677 CD GLU A 216 35.637 53.492 37.941 1.00 34.02 A C
ATOM 1678 OE1 GLU A 216 36.824 53.286 37.609 1.00 31.93 A O
ATOM 1679 OE2 GLU A 216 34.868 54.236 37.285 1.00 35.33 A O
ATOM 1680 C GLU A 216 36.447 52.971 42.846 1.00 17.32 A C
ATOM 1681 O GLU A 216 37.245 52.188 43.363 1.00 16.80 A O
ATOM 1682 N TYR A 217 36.352 54.248 43.204 1.00 16.20 A N
ATOM 1683 CA TYR A 217 37.200 54.818 44.244 1.00 16.23 A C
ATOM 1684 CB TYR A 217 36.900 56.308 44.432 1.00 14.73 A C
ATOM 1685 CG TYR A 217 37.693 56.942 45.557 1.00 17.55 A C
ATOM 1686 CD1 TYR A 217 39.053 57.202 45.418 1.00 18.17 A C
ATOM 1687 CE1 TYR A 217 39.797 57.738 46.475 1.00 18.51 A C
ATOM 1688 CD2 TYR A 217 37.089 57.234 46.780 1.00 16.61 A C
ATOM 1689 CE2 TYR A 217 37.815 57.765 47.836 1.00 17.74 A C
ATOM 1690 CZ TYR A 217 39.168 58.014 47.680 1.00 19.47 A C
ATOM 1691 OH TYR A 217 39.891 58.526 48.735 1.00 18.42 A O
ATOM 1692 C TYR A 217 37.041 54.116 45.584 1.00 16.31 A C

Figure 5EE

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ATOM  1693  O   TYR A 217     38.028  53.715  46.199  1.00 16.78    A   O
ATOM  1694  N   LEU A 218     35.798  53.995  46.045  1.00 15.56    A   N
ATOM  1695  CA  LEU A 218     35.509  53.353  47.324  1.00 18.16    A   C
ATOM  1696  CB  LEU A 218     33.993  53.344  47.575  1.00 15.21    A   C
ATOM  1697  CG  LEU A 218     33.321  54.705  47.799  1.00 15.27    A   C
ATOM  1698  CD1 LEU A 218     31.798  54.546  47.756  1.00 14.34    A   C
ATOM  1699  CD2 LEU A 218     33.775  55.294  49.129  1.00 13.25    A   C
ATOM  1700  C   LEU A 218     36.058  51.926  47.402  1.00 18.45    A   C
ATOM  1701  O   LEU A 218     36.648  51.531  48.409  1.00 18.06    A   O
ATOM  1702  N   GLN A 219     35.871  51.150  46.341  1.00 17.77    A   N
ATOM  1703  CA  GLN A 219     36.367  49.778  46.335  1.00 19.66    A   C
ATOM  1704  CB  GLN A 219     36.042  49.097  45.005  1.00 18.42    A   C
ATOM  1705  CG  GLN A 219     34.577  49.147  44.645  1.00 17.80    A   C
ATOM  1706  CD  GLN A 219     34.282  48.496  43.318  1.00 17.89    A   C
ATOM  1707  OE1 GLN A 219     35.071  48.596  42.372  1.00 18.96    A   O
ATOM  1708  NE2 GLN A 219     33.134  47.837  43.228  1.00 13.87    A   N
ATOM  1709  C   GLN A 219     37.876  49.740  46.567  1.00 19.63    A   C
ATOM  1710  O   GLN A 219     38.368  48.964  47.380  1.00 19.95    A   O
ATOM  1711  N   GLN A 220     38.605  50.593  45.859  1.00 21.16    A   N
ATOM  1712  CA  GLN A 220     40.057  50.621  45.992  1.00 24.11    A   C
ATOM  1713  CB  GLN A 220     40.681  51.372  44.811  1.00 25.85    A   C
ATOM  1714  CG  GLN A 220     42.197  51.445  44.885  1.00 34.94    A   C
ATOM  1715  CD  GLN A 220     42.830  51.975  43.615  1.00 40.03    A   C
ATOM  1716  OE1 GLN A 220     44.050  52.152  43.548  1.00 44.37    A   O
ATOM  1717  NE2 GLN A 220     42.010  52.227  42.598  1.00 41.95    A   N
ATOM  1718  C   GLN A 220     40.534  51.242  47.304  1.00 22.63    A   C
ATOM  1719  O   GLN A 220     41.275  50.617  48.062  1.00 21.00    A   O
ATOM  1720  N   LYS A 221     40.104  52.472  47.564  1.00 21.71    A   N
ATOM  1721  CA  LYS A 221     40.503  53.194  48.770  1.00 22.37    A   C
ATOM  1722  CB  LYS A 221     39.830  54.570  48.795  1.00 21.53    A   C
ATOM  1723  CG  LYS A 221     39.984  55.325  50.111  1.00 25.31    A   C
ATOM  1724  CD  LYS A 221     41.443  55.615  50.439  1.00 26.19    A   C
ATOM  1725  CE  LYS A 221     41.579  56.244  51.818  1.00 29.00    A   C
ATOM  1726  NZ  LYS A 221     42.999  56.511  52.159  1.00 29.71    A   N
ATOM  1727  C   LYS A 221     40.221  52.464  50.084  1.00 22.42    A   C
ATOM  1728  O   LYS A 221     41.090  52.376  50.953  1.00 21.37    A   O
ATOM  1729  N   TYR A 222     39.005  51.950  50.229  1.00 20.94    A   N
ATOM  1730  CA  TYR A 222     38.616  51.250  51.442  1.00 21.75    A   C
ATOM  1731  CB  TYR A 222     37.251  51.762  51.903  1.00 22.02    A   C
ATOM  1732  CG  TYR A 222     37.277  53.247  52.204  1.00 20.42    A   C
ATOM  1733  CD1 TYR A 222     36.737  54.178  51.314  1.00 18.91    A   C
ATOM  1734  CE1 TYR A 222     36.866  55.549  51.545  1.00 20.88    A   C
ATOM  1735  CD2 TYR A 222     37.938  53.725  53.336  1.00 21.77    A   C
ATOM  1736  CE2 TYR A 222     38.074  55.080  53.577  1.00 19.97    A   C
ATOM  1737  CZ  TYR A 222     37.540  55.988  52.679  1.00 20.71    A   C
ATOM  1738  OH  TYR A 222     37.705  57.330  52.909  1.00 16.95    A   O
ATOM  1739  C   TYR A 222     38.637  49.731  51.350  1.00 21.67    A   C
ATOM  1740  O   TYR A 222     38.112  49.040  52.226  1.00 20.83    A   O
ATOM  1741  N   ALA A 223     39.264  49.219  50.292  1.00 21.20    A   N
ATOM  1742  CA  ALA A 223     39.408  47.774  50.077  1.00 22.92    A   C
ATOM  1743  CB  ALA A 223     40.466  47.204  50.984  1.00 23.23    A   C
ATOM  1744  C   ALA A 223     38.105  47.055  50.330  1.00 23.19    A   C
ATOM  1745  O   ALA A 223     38.024  46.162  51.180  1.00 20.95    A   O
ATOM  1746  N   LEU A 224     37.088  47.426  49.565  1.00 25.19    A   N
ATOM  1747  CA  LEU A 224     35.759  46.839  49.692  1.00 24.53    A   C
ATOM  1748  CB  LEU A 224     34.703  47.937  49.609  1.00 22.99    A   C
ATOM  1749  CG  LEU A 224     34.869  49.090  50.607  1.00 21.68    A   C
ATOM  1750  CD1 LEU A 224     33.731  50.099  50.443  1.00 22.66    A   C
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Figure 5FF

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ATOM  1751  CD2 LEU A 224     34.875  48.531  52.022  1.00 23.83      A   C
ATOM  1752  C   LEU A 224     35.576  45.852  48.551  1.00 24.10      A   C
ATOM  1753  O   LEU A 224     35.569  46.259  47.400  1.00 22.11      A   O
ATOM  1754  N   LYS A 225     35.368  44.572  48.866  1.00 26.47      A   N
ATOM  1755  CA  LYS A 225     35.212  43.532  47.846  1.00 25.75      A   C
ATOM  1756  CB  LYS A 225     35.880  42.233  48.331  1.00 26.74      A   C
ATOM  1757  CG  LYS A 225     37.358  42.380  48.669  1.00 28.32      A   C
ATOM  1758  CD  LYS A 225     38.185  42.652  47.421  1.00 31.42      A   C
ATOM  1759  CE  LYS A 225     38.157  41.461  46.478  1.00 32.69      A   C
ATOM  1760  NZ  LYS A 225     39.003  41.698  45.284  1.00 34.46      A   N
ATOM  1761  C   LYS A 225     33.803  43.213  47.340  1.00 24.95      A   C
ATOM  1762  O   LYS A 225     33.568  42.125  46.819  1.00 29.54      A   O
ATOM  1763  N   ASN A 226     32.870  44.143  47.489  1.00 23.13      A   N
ATOM  1764  CA  ASN A 226     31.498  43.938  47.019  1.00 20.01      A   C
ATOM  1765  CB  ASN A 226     31.469  43.729  45.500  1.00 19.42      A   C
ATOM  1766  CG  ASN A 226     32.287  44.755  44.751  1.00 23.12      A   C
ATOM  1767  OD1 ASN A 226     33.342  44.439  44.190  1.00 20.38      A   O
ATOM  1768  ND2 ASN A 226     31.814  45.995  44.743  1.00 16.65      A   N
ATOM  1769  C   ASN A 226     30.800  42.740  47.662  1.00 21.21      A   C
ATOM  1770  O   ASN A 226     30.086  41.999  46.981  1.00 18.29      A   O
ATOM  1771  N   ASN A 227     30.984  42.551  48.963  1.00 22.29      A   N
ATOM  1772  CA  ASN A 227     30.362  41.421  49.641  1.00 22.96      A   C
ATOM  1773  CB  ASN A 227     31.438  40.462  50.163  1.00 22.46      A   C
ATOM  1774  CG  ASN A 227     32.503  41.165  50.982  1.00 21.07      A   C
ATOM  1775  OD1 ASN A 227     32.223  42.137  51.679  1.00 19.99      A   O
ATOM  1776  ND2 ASN A 227     33.733  40.659  50.916  1.00 19.44      A   N
ATOM  1777  C   ASN A 227     29.428  41.805  50.783  1.00 24.57      A   C
ATOM  1778  O   ASN A 227     29.198  41.005  51.690  1.00 21.91      A   O
ATOM  1779  N   ALA A 228     28.891  43.021  50.741  1.00 23.23      A   N
ATOM  1780  CA  ALA A 228     27.969  43.481  51.776  1.00 26.14      A   C
ATOM  1781  CB  ALA A 228     27.806  45.001  51.699  1.00 22.82      A   C
ATOM  1782  C   ALA A 228     26.611  42.793  51.596  1.00 26.93      A   C
ATOM  1783  O   ALA A 228     26.405  42.077  50.619  1.00 26.75      A   O
ATOM  1784  N   CYS A 229     25.698  43.016  52.541  1.00 29.94      A   N
ATOM  1785  CA  CYS A 229     24.359  42.425  52.508  1.00 34.05      A   C
ATOM  1786  CB  CYS A 229     23.438  43.143  53.508  1.00 36.45      A   C
ATOM  1787  SG  CYS A 229     23.886  42.897  55.243  1.00 48.21      A   S
ATOM  1788  C   CYS A 229     23.730  42.476  51.124  1.00 35.31      A   C
ATOM  1789  O   CYS A 229     23.882  43.451  50.399  1.00 35.27      A   O
ATOM  1790  N   THR A 230     23.030  41.412  50.757  1.00 38.04      A   N
ATOM  1791  CA  THR A 230     22.378  41.380  49.466  1.00 40.97      A   C
ATOM  1792  CB  THR A 230     21.965  39.958  49.076  1.00 42.40      A   C
ATOM  1793  OG1 THR A 230     21.273  39.335  50.163  1.00 45.09      A   O
ATOM  1794  CG2 THR A 230     23.190  39.148  48.730  1.00 43.15      A   C
ATOM  1795  C   THR A 230     21.150  42.269  49.476  1.00 41.97      A   C
ATOM  1796  O   THR A 230     20.887  42.971  48.493  1.00 42.37      A   O
ATOM  1797  N   PHE A 231     20.376  42.232  50.552  1.00 42.74      A   N
ATOM  1798  CA  PHE A 231     19.230  43.108  50.576  1.00 43.96      A   C
ATOM  1799  CB  PHE A 231     17.938  42.321  50.366  1.00 49.35      A   C
ATOM  1800  CG  PHE A 231     17.721  41.990  48.907  1.00 55.66      A   C
ATOM  1801  CD1 PHE A 231     18.494  41.004  48.306  1.00 58.70      A   C
ATOM  1802  CD2 PHE A 231     16.903  42.785  48.088  1.00 58.59      A   C
ATOM  1803  CE1 PHE A 231     18.483  40.801  46.922  1.00 60.69      A   C
ATOM  1804  CE2 PHE A 231     16.879  42.597  46.701  1.00 60.58      A   C
ATOM  1805  CZ  PHE A 231     17.668  41.604  46.113  1.00 60.92      A   C
ATOM  1806  C   PHE A 231     19.335  43.912  51.838  1.00 40.83      A   C
ATOM  1807  O   PHE A 231     18.811  43.567  52.886  1.00 42.69      A   O
ATOM  1808  N   PRO A 232     20.153  44.975  51.722  1.00 35.76      A   N
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Figure 5GG

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ATOM  1809 CD  PRO A 232     20.672  45.196  50.347  1.00 35.27    A   C
ATOM  1810 CA  PRO A 232     20.579  46.028  52.651  1.00 32.93    A   C
ATOM  1811 CB  PRO A 232     21.689  46.764  51.874  1.00 32.41    A   C
ATOM  1812 CG  PRO A 232     21.363  46.497  50.424  1.00 32.47    A   C
ATOM  1813 C   PRO A 232     19.457  46.929  53.137  1.00 29.06    A   C
ATOM  1814 O   PRO A 232     18.456  47.146  52.452  1.00 27.86    A   O
ATOM  1815 N   LYS A 233     19.630  47.440  54.346  1.00 27.89    A   N
ATOM  1816 CA  LYS A 233     18.645  48.314  54.943  1.00 25.66    A   C
ATOM  1817 CB  LYS A 233     18.682  48.188  56.464  1.00 29.61    A   C
ATOM  1818 CG  LYS A 233     18.178  46.843  56.973  1.00 34.08    A   C
ATOM  1819 CD  LYS A 233     18.086  46.829  58.491  1.00 40.01    A   C
ATOM  1820 CE  LYS A 233     19.454  46.996  59.139  1.00 41.92    A   C
ATOM  1821 NZ  LYS A 233     19.351  47.038  60.626  1.00 44.78    A   N
ATOM  1822 C   LYS A 233     18.945  49.739  54.524  1.00 23.25    A   C
ATOM  1823 O   LYS A 233     20.042  50.248  54.738  1.00 20.72    A   O
ATOM  1824 N   VAL A 234     17.959  50.374  53.909  1.00 21.94    A   N
ATOM  1825 CA  VAL A 234     18.122  51.742  53.457  1.00 18.96    A   C
ATOM  1826 CB  VAL A 234     18.171  51.809  51.927  1.00 18.07    A   C
ATOM  1827 CG1 VAL A 234     18.407  53.242  51.484  1.00 15.91    A   C
ATOM  1828 CG2 VAL A 234     19.265  50.884  51.403  1.00 19.03    A   C
ATOM  1829 C   VAL A 234     16.982  52.622  53.945  1.00 19.45    A   C
ATOM  1830 O   VAL A 234     15.810  52.291  53.775  1.00 18.84    A   O
ATOM  1831 N   GLU A 235     17.332  53.749  54.550  1.00 18.70    A   N
ATOM  1832 CA  GLU A 235     16.333  54.682  55.044  1.00 19.65    A   C
ATOM  1833 CB  GLU A 235     16.584  55.029  56.513  1.00 20.87    A   C
ATOM  1834 CG  GLU A 235     16.619  53.849  57.461  1.00 24.25    A   C
ATOM  1835 CD  GLU A 235     16.762  54.287  58.908  1.00 26.71    A   C
ATOM  1836 OE1 GLU A 235     16.924  53.412  59.782  1.00 30.95    A   O
ATOM  1837 OE2 GLU A 235     16.710  55.509  59.174  1.00 28.58    A   O
ATOM  1838 C   GLU A 235     16.433  55.957  54.226  1.00 19.63    A   C
ATOM  1839 O   GLU A 235     17.522  56.339  53.793  1.00 19.08    A   O
ATOM  1840 N   PHE A 236     15.295  56.608  54.008  1.00 16.22    A   N
ATOM  1841 CA  PHE A 236     15.281  57.850  53.260  1.00 15.50    A   C
ATOM  1842 CB  PHE A 236     14.454  57.703  51.985  1.00 16.22    A   C
ATOM  1843 CG  PHE A 236     15.028  56.712  51.008  1.00 16.49    A   C
ATOM  1844 CD1 PHE A 236     14.734  55.352  51.117  1.00 14.80    A   C
ATOM  1845 CD2 PHE A 236     15.906  57.131  50.011  1.00 16.20    A   C
ATOM  1846 CE1 PHE A 236     15.311  54.423  50.249  1.00 16.35    A   C
ATOM  1847 CE2 PHE A 236     16.488  56.213  49.140  1.00 16.85    A   C
ATOM  1848 CZ  PHE A 236     16.191  54.857  49.258  1.00 18.08    A   C
ATOM  1849 C   PHE A 236     14.725  58.953  54.150  1.00 17.81    A   C
ATOM  1850 O   PHE A 236     13.669  58.808  54.771  1.00 17.48    A   O
ATOM  1851 N   HIS A 237     15.473  60.043  54.238  1.00 14.01    A   N
ATOM  1852 CA  HIS A 237     15.077  61.178  55.050  1.00 13.85    A   C
ATOM  1853 CB  HIS A 237     15.976  61.261  56.282  1.00 16.76    A   C
ATOM  1854 CG  HIS A 237     15.871  60.068  57.183  1.00 20.30    A   C
ATOM  1855 CD2 HIS A 237     16.529  58.884  57.176  1.00 22.69    A   C
ATOM  1856 ND1 HIS A 237     14.963  59.994  58.216  1.00 21.64    A   N
ATOM  1857 CE1 HIS A 237     15.065  58.816  58.808  1.00 24.58    A   C
ATOM  1858 NE2 HIS A 237     16.008  58.123  58.196  1.00 24.02    A   N
ATOM  1859 C   HIS A 237     15.240  62.421  54.190  1.00 12.98    A   C
ATOM  1860 O   HIS A 237     15.960  62.402  53.199  1.00 14.24    A   O
ATOM  1861 N   ALA A 238     14.573  63.500  54.571  1.00 14.25    A   N
ATOM  1862 CA  ALA A 238     14.656  64.745  53.822  1.00 14.74    A   C
ATOM  1863 CB  ALA A 238     13.867  64.622  52.523  1.00 13.87    A   C
ATOM  1864 C   ALA A 238     14.105  65.889  54.662  1.00 16.80    A   C
ATOM  1865 O   ALA A 238     13.416  65.662  55.659  1.00 13.41    A   O
ATOM  1866 N   SER A 239     14.419  67.118  54.265  1.00 16.83    A   N
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Figure 5HH

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ATOM  1867  CA  SER A 239     13.934  68.289  54.982  1.00 15.86      A   C
ATOM  1868  CB  SER A 239     14.874  69.472  54.749  1.00 17.78      A   C
ATOM  1869  OG  SER A 239     15.235  69.570  53.382  1.00 15.31      A   O
ATOM  1870  C   SER A 239     12.526  68.628  54.501  1.00 18.27      A   C
ATOM  1871  O   SER A 239     11.851  69.475  55.081  1.00 19.09      A   O
ATOM  1872  N   GLY A 240     12.093  67.950  53.440  1.00 19.12      A   N
ATOM  1873  CA  GLY A 240     10.764  68.172  52.891  1.00 18.85      A   C
ATOM  1874  C   GLY A 240     10.400  67.108  51.872  1.00 20.08      A   C
ATOM  1875  O   GLY A 240     11.262  66.321  51.462  1.00 19.84      A   O
ATOM  1876  N   ASP A 241      9.134  67.065  51.464  1.00 17.58      A   N
ATOM  1877  CA  ASP A 241      8.692  66.077  50.481  1.00 19.46      A   C
ATOM  1878  CB  ASP A 241      9.150  66.501  49.083  1.00 21.27      A   C
ATOM  1879  CG  ASP A 241      8.429  67.738  48.587  1.00 23.85      A   C
ATOM  1880  OD1 ASP A 241      7.247  67.610  48.206  1.00 26.32      A   O
ATOM  1881  OD2 ASP A 241      9.038  68.833  48.591  1.00 21.42      A   O
ATOM  1882  C   ASP A 241      9.257  64.694  50.803  1.00 16.99      A   C
ATOM  1883  O   ASP A 241      9.731  63.987  49.913  1.00 17.49      A   O
ATOM  1884  N   VAL A 242      9.208  64.316  52.076  1.00 15.93      A   N
ATOM  1885  CA  VAL A 242      9.737  63.025  52.516  1.00 14.13      A   C
ATOM  1886  CB  VAL A 242      9.894  62.990  54.052  1.00 17.19      A   C
ATOM  1887  CG1 VAL A 242     10.671  61.740  54.469  1.00 16.23      A   C
ATOM  1888  CG2 VAL A 242     10.612  64.248  54.523  1.00 18.97      A   C
ATOM  1889  C   VAL A 242      8.849  61.864  52.082  1.00 15.60      A   C
ATOM  1890  O   VAL A 242      9.341  60.808  51.660  1.00 12.78      A   O
ATOM  1891  N   ILE A 243      7.540  62.057  52.209  1.00 14.41      A   N
ATOM  1892  CA  ILE A 243      6.577  61.045  51.803  1.00 16.25      A   C
ATOM  1893  CB  ILE A 243      5.125  61.549  52.007  1.00 18.10      A   C
ATOM  1894  CG2 ILE A 243      4.123  60.554  51.414  1.00 20.99      A   C
ATOM  1895  CG1 ILE A 243      4.858  61.747  53.502  1.00 21.18      A   C
ATOM  1896  CD1 ILE A 243      3.485  62.293  53.817  1.00 20.78      A   C
ATOM  1897  C   ILE A 243      6.833  60.787  50.324  1.00 15.05      A   C
ATOM  1898  O   ILE A 243      6.885  59.639  49.878  1.00 16.76      A   O
ATOM  1899  N   TRP A 244      7.005  61.868  49.569  1.00 13.24      A   N
ATOM  1900  CA  TRP A 244      7.270  61.768  48.142  1.00 15.52      A   C
ATOM  1901  CB  TRP A 244      7.343  63.164  47.523  1.00 13.47      A   C
ATOM  1902  CG  TRP A 244      7.510  63.151  46.036  1.00 18.87      A   C
ATOM  1903  CD2 TRP A 244      8.732  63.342  45.312  1.00 17.48      A   C
ATOM  1904  CE2 TRP A 244      8.426  63.232  43.940  1.00 18.22      A   C
ATOM  1905  CE3 TRP A 244     10.057  63.594  45.693  1.00 17.59      A   C
ATOM  1906  CD1 TRP A 244      6.538  62.938  45.099  1.00 18.15      A   C
ATOM  1907  NE1 TRP A 244      7.083  62.988  43.835  1.00 18.29      A   N
ATOM  1908  CZ2 TRP A 244      9.399  63.366  42.943  1.00 20.22      A   C
ATOM  1909  CZ3 TRP A 244     11.024  63.727  44.702  1.00 18.36      A   C
ATOM  1910  CH2 TRP A 244     10.688  63.611  43.342  1.00 18.43      A   C
ATOM  1911  C   TRP A 244      8.590  61.042  47.891  1.00 14.64      A   C
ATOM  1912  O   TRP A 244      8.670  60.149  47.044  1.00 16.51      A   O
ATOM  1913  N   LEU A 245      9.628  61.436  48.623  1.00 13.56      A   N
ATOM  1914  CA  LEU A 245     10.941  60.814  48.459  1.00 12.19      A   C
ATOM  1915  CB  LEU A 245     11.946  61.416  49.444  1.00 11.28      A   C
ATOM  1916  CG  LEU A 245     13.379  60.875  49.342  1.00 11.24      A   C
ATOM  1917  CD1 LEU A 245     13.988  61.289  48.009  1.00 11.74      A   C
ATOM  1918  CD2 LEU A 245     14.223  61.407  50.490  1.00 10.22      A   C
ATOM  1919  C   LEU A 245     10.862  59.301  48.661  1.00 14.05      A   C
ATOM  1920  O   LEU A 245     11.439  58.537  47.884  1.00 12.33      A   O
ATOM  1921  N   GLU A 246     10.144  58.870  49.698  1.00 14.68      A   N
ATOM  1922  CA  GLU A 246     10.000  57.441  49.980  1.00 16.30      A   C
ATOM  1923  CB  GLU A 246      9.198  57.213  51.267  1.00 16.70      A   C
ATOM  1924  CG  GLU A 246      9.938  57.637  52.521  1.00 23.08      A   C
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Figure 5II

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ATOM  1925  CD  GLU A 246      9.544  56.818  53.737  1.00 25.63      A   C
ATOM  1926  OE1 GLU A 246      8.335  56.577  53.927  1.00 24.93      A   O
ATOM  1927  OE2 GLU A 246     10.444  56.423  54.508  1.00 27.10      A   O
ATOM  1928  C   GLU A 246      9.324  56.714  48.828  1.00 15.72      A   C
ATOM  1929  O   GLU A 246      9.691  55.589  48.494  1.00 15.40      A   O
ATOM  1930  N   ARG A 247      8.326  57.359  48.235  1.00 16.57      A   N
ATOM  1931  CA  ARG A 247      7.611  56.790  47.105  1.00 18.74      A   C
ATOM  1932  CB  ARG A 247      6.445  57.710  46.711  1.00 23.10      A   C
ATOM  1933  CG  ARG A 247      5.875  57.451  45.325  1.00 32.32      A   C
ATOM  1934  CD  ARG A 247      4.561  58.204  45.114  1.00 40.32      A   C
ATOM  1935  NE  ARG A 247      4.084  58.117  43.733  1.00 47.44      A   N
ATOM  1936  CZ  ARG A 247      4.569  58.835  42.722  1.00 49.78      A   C
ATOM  1937  NH1 ARG A 247      5.548  59.705  42.931  1.00 51.70      A   N
ATOM  1938  NH2 ARG A 247      4.079  58.682  41.497  1.00 52.43      A   N
ATOM  1939  C   ARG A 247      8.594  56.630  45.941  1.00 17.54      A   C
ATOM  1940  O   ARG A 247      8.654  55.578  45.299  1.00 14.31      A   O
ATOM  1941  N   GLN A 248      9.375  57.672  45.677  1.00 15.93      A   N
ATOM  1942  CA  GLN A 248     10.350  57.608  44.598  1.00 16.24      A   C
ATOM  1943  CB  GLN A 248     11.120  58.929  44.485  1.00 17.33      A   C
ATOM  1944  CG  GLN A 248     10.267  60.119  44.047  1.00 16.22      A   C
ATOM  1945  CD  GLN A 248      9.552  59.879  42.725  1.00 22.44      A   C
ATOM  1946  OE1 GLN A 248     10.184  59.627  41.694  1.00 22.85      A   O
ATOM  1947  NE2 GLN A 248      8.225  59.958  42.749  1.00 24.90      A   N
ATOM  1948  C   GLN A 248     11.324  56.453  44.815  1.00 15.90      A   C
ATOM  1949  O   GLN A 248     11.705  55.768  43.866  1.00 16.87      A   O
ATOM  1950  N   ALA A 249     11.720  56.231  46.065  1.00 15.92      A   N
ATOM  1951  CA  ALA A 249     12.644  55.146  46.384  1.00 15.55      A   C
ATOM  1952  CB  ALA A 249     13.015  55.191  47.857  1.00 16.80      A   C
ATOM  1953  C   ALA A 249     12.032  53.789  46.041  1.00 16.47      A   C
ATOM  1954  O   ALA A 249     12.685  52.943  45.426  1.00 16.21      A   O
ATOM  1955  N   LYS A 250     10.779  53.582  46.438  1.00 16.38      A   N
ATOM  1956  CA  LYS A 250     10.102  52.316  46.159  1.00 18.81      A   C
ATOM  1957  CB  LYS A 250      8.750  52.258  46.880  1.00 20.86      A   C
ATOM  1958  CG  LYS A 250      8.843  52.132  48.394  1.00 26.84      A   C
ATOM  1959  CD  LYS A 250      7.488  51.745  48.988  1.00 31.08      A   C
ATOM  1960  CE  LYS A 250      7.554  51.607  50.507  1.00 31.43      A   C
ATOM  1961  NZ  LYS A 250      7.896  52.899  51.156  1.00 29.87      A   N
ATOM  1962  C   LYS A 250      9.884  52.121  44.661  1.00 18.41      A   C
ATOM  1963  O   LYS A 250     10.073  51.024  44.125  1.00 15.17      A   O
ATOM  1964  N   GLU A 251      9.493  53.200  43.992  1.00 15.62      A   N
ATOM  1965  CA  GLU A 251      9.224  53.167  42.562  1.00 18.32      A   C
ATOM  1966  CB  GLU A 251      8.586  54.486  42.119  1.00 20.33      A   C
ATOM  1967  CG  GLU A 251      7.205  54.758  42.692  1.00 23.48      A   C
ATOM  1968  CD  GLU A 251      6.106  54.036  41.936  1.00 25.23      A   C
ATOM  1969  OE1 GLU A 251      6.415  53.361  40.932  1.00 28.49      A   O
ATOM  1970  OE2 GLU A 251      4.932  54.152  42.341  1.00 25.47      A   O
ATOM  1971  C   GLU A 251     10.448  52.921  41.694  1.00 20.06      A   C
ATOM  1972  O   GLU A 251     10.398  52.121  40.763  1.00 17.23      A   O
ATOM  1973  N   TRP A 252     11.547  53.606  41.997  1.00 19.52      A   N
ATOM  1974  CA  TRP A 252     12.748  53.489  41.175  1.00 20.14      A   C
ATOM  1975  CB  TRP A 252     13.276  54.885  40.832  1.00 18.05      A   C
ATOM  1976  CG  TRP A 252     12.305  55.710  40.043  1.00 18.22      A   C
ATOM  1977  CD2 TRP A 252     12.039  55.607  38.640  1.00 20.57      A   C
ATOM  1978  CE2 TRP A 252     11.017  56.533  38.339  1.00 20.85      A   C
ATOM  1979  CE3 TRP A 252     12.564  54.818  37.607  1.00 21.87      A   C
ATOM  1980  CD1 TRP A 252     11.460  56.669  40.523  1.00 17.88      A   C
ATOM  1981  NE1 TRP A 252     10.683  57.168  39.508  1.00 17.77      A   N
ATOM  1982  CZ2 TRP A 252     10.506  56.697  37.041  1.00 22.03      A   C
```

Figure 5JJ

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ATOM  1983 CZ3 TRP A 252     12.055  54.978  36.314  1.00 21.57    A   C
ATOM  1984 CH2 TRP A 252     11.036  55.913  36.045  1.00 22.86    A   C
ATOM  1985 C   TRP A 252     13.902  52.641  41.688  1.00 22.39    A   C
ATOM  1986 O   TRP A 252     14.680  52.122  40.886  1.00 23.72    A   O
ATOM  1987 N   LEU A 253     14.024  52.504  43.003  1.00 22.18    A   N
ATOM  1988 CA  LEU A 253     15.106  51.717  43.588  1.00 25.35    A   C
ATOM  1989 CB  LEU A 253     15.809  52.524  44.680  1.00 20.44    A   C
ATOM  1990 CG  LEU A 253     16.355  53.904  44.285  1.00 21.92    A   C
ATOM  1991 CD1 LEU A 253     16.785  54.649  45.532  1.00 18.63    A   C
ATOM  1992 CD2 LEU A 253     17.530  53.758  43.316  1.00 20.79    A   C
ATOM  1993 C   LEU A 253     14.583  50.401  44.168  1.00 29.73    A   C
ATOM  1994 O   LEU A 253     15.357  49.570  44.647  1.00 31.04    A   O
ATOM  1995 N   LYS A 254     13.267  50.219  44.121  1.00 33.91    A   N
ATOM  1996 CA  LYS A 254     12.638  49.007  44.631  1.00 39.79    A   C
ATOM  1997 CB  LYS A 254     13.102  47.795  43.812  1.00 43.18    A   C
ATOM  1998 CG  LYS A 254     12.330  46.518  44.102  1.00 51.27    A   C
ATOM  1999 CD  LYS A 254     12.747  45.377  43.181  1.00 56.67    A   C
ATOM  2000 CE  LYS A 254     11.928  44.121  43.464  1.00 59.29    A   C
ATOM  2001 NZ  LYS A 254     10.463  44.368  43.307  1.00 62.20    A   N
ATOM  2002 C   LYS A 254     12.967  48.805  46.110  1.00 41.24    A   C
ATOM  2003 O   LYS A 254     13.111  47.678  46.586  1.00 42.02    A   O
ATOM  2004 N   LEU A 255     13.091  49.911  46.834  1.00 42.21    A   N
ATOM  2005 CA  LEU A 255     13.396  49.856  48.255  1.00 43.88    A   C
ATOM  2006 CB  LEU A 255     14.643  50.687  48.560  1.00 41.85    A   C
ATOM  2007 CG  LEU A 255     15.934  50.186  47.910  1.00 40.40    A   C
ATOM  2008 CD1 LEU A 255     17.065  51.143  48.229  1.00 40.11    A   C
ATOM  2009 CD2 LEU A 255     16.258  48.788  48.412  1.00 39.40    A   C
ATOM  2010 C   LEU A 255     12.211  50.365  49.070  1.00 46.21    A   C
ATOM  2011 O   LEU A 255     12.350  51.427  49.715  1.00 47.30    A   O
ATOM  2012 OXT LEU A 255     11.152  49.696  49.044  1.00 48.09    A   O
ATOM  2013 CB  MET B   1      3.272 103.508  55.905  1.00 23.27    B   C
ATOM  2014 CG  MET B   1      3.026 102.116  56.484  1.00 25.31    B   C
ATOM  2015 SD  MET B   1      1.613 101.253  55.747  1.00 29.32    B   S
ATOM  2016 CE  MET B   1      0.239 102.076  56.594  1.00 27.48    B   C
ATOM  2017 C   MET B   1      5.739 103.357  56.203  1.00 22.82    B   C
ATOM  2018 O   MET B   1      6.391 103.503  55.166  1.00 21.44    B   O
ATOM  2019 N   MET B   1      4.661 105.565  55.875  1.00 22.28    B   N
ATOM  2020 CA  MET B   1      4.509 104.211  56.478  1.00 22.89    B   C
ATOM  2021 N   LYS B   2      6.057 102.479  57.148  1.00 22.63    B   N
ATOM  2022 CA  LYS B   2      7.185 101.568  57.010  1.00 21.27    B   C
ATOM  2023 CB  LYS B   2      8.060 101.591  58.260  1.00 21.29    B   C
ATOM  2024 CG  LYS B   2      9.273 100.675  58.156  1.00 18.62    B   C
ATOM  2025 CD  LYS B   2     10.097 100.705  59.419  1.00 18.80    B   C
ATOM  2026 CE  LYS B   2     11.414  99.983  59.213  1.00 19.94    B   C
ATOM  2027 NZ  LYS B   2     12.203  99.908  60.474  1.00 21.20    B   N
ATOM  2028 C   LYS B   2      6.610 100.169  56.822  1.00 19.67    B   C
ATOM  2029 O   LYS B   2      5.903  99.661  57.692  1.00 20.03    B   O
ATOM  2030 N   ILE B   3      6.915  99.545  55.689  1.00 18.60    B   N
ATOM  2031 CA  ILE B   3      6.395  98.213  55.410  1.00 16.13    B   C
ATOM  2032 CB  ILE B   3      5.409  98.250  54.232  1.00 18.20    B   C
ATOM  2033 CG2 ILE B   3      4.281  99.237  54.516  1.00 15.72    B   C
ATOM  2034 CG1 ILE B   3      6.156  98.669  52.964  1.00 17.99    B   C
ATOM  2035 CD1 ILE B   3      5.909  97.772  51.772  1.00 20.13    B   C
ATOM  2036 C   ILE B   3      7.476  97.190  55.062  1.00 17.01    B   C
ATOM  2037 O   ILE B   3      8.637  97.535  54.820  1.00 13.35    B   O
ATOM  2038 N   GLY B   4      7.072  95.924  55.046  1.00 15.79    B   N
ATOM  2039 CA  GLY B   4      7.982  94.859  54.678  1.00 13.12    B   C
ATOM  2040 C   GLY B   4      7.474  94.217  53.401  1.00 12.84    B   C
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Figure 5KK

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ATOM  2041  O   GLY B  4     6.271  94.248  53.123  1.00 12.27    B   O
ATOM  2042  N   VAL B  5     8.387  93.670  52.602  1.00 11.41    B   N
ATOM  2043  CA  VAL B  5     8.024  92.982  51.362  1.00 12.46    B   C
ATOM  2044  CB  VAL B  5     8.471  93.755  50.092  1.00 11.43    B   C
ATOM  2045  CG1 VAL B  5     8.281  92.886  48.860  1.00 10.57    B   C
ATOM  2046  CG2 VAL B  5     7.646  95.026  49.938  1.00 13.41    B   C
ATOM  2047  C   VAL B  5     8.745  91.641  51.404  1.00 11.84    B   C
ATOM  2048  O   VAL B  5     9.964  91.591  51.565  1.00 13.84    B   O
ATOM  2049  N   PHE B  6     7.989  90.559  51.277  1.00 11.52    B   N
ATOM  2050  CA  PHE B  6     8.571  89.222  51.330  1.00 12.00    B   C
ATOM  2051  CB  PHE B  6     7.930  88.429  52.471  1.00 14.01    B   C
ATOM  2052  CG  PHE B  6     8.313  86.975  52.485  1.00 15.68    B   C
ATOM  2053  CD1 PHE B  6     9.650  86.598  52.576  1.00 15.79    B   C
ATOM  2054  CD2 PHE B  6     7.340  85.983  52.403  1.00 17.28    B   C
ATOM  2055  CE1 PHE B  6    10.017  85.251  52.584  1.00 15.22    B   C
ATOM  2056  CE2 PHE B  6     7.699  84.628  52.411  1.00 18.59    B   C
ATOM  2057  CZ  PHE B  6     9.044  84.268  52.502  1.00 15.23    B   C
ATOM  2058  C   PHE B  6     8.440  88.410  50.046  1.00 12.99    B   C
ATOM  2059  O   PHE B  6     7.396  88.412  49.400  1.00 13.52    B   O
ATOM  2060  N   ASP B  7     9.512  87.707  49.695  1.00 13.22    B   N
ATOM  2061  CA  ASP B  7     9.533  86.839  48.523  1.00 12.28    B   C
ATOM  2062  CB  ASP B  7     9.914  87.600  47.254  1.00 12.10    B   C
ATOM  2063  CG  ASP B  7     9.838  86.727  46.018  1.00 11.16    B   C
ATOM  2064  OD1 ASP B  7     8.773  86.111  45.800  1.00 11.05    B   O
ATOM  2065  OD2 ASP B  7    10.835  86.652  45.265  1.00 15.46    B   O
ATOM  2066  C   ASP B  7    10.544  85.730  48.749  1.00 12.97    B   C
ATOM  2067  O   ASP B  7    11.402  85.831  49.626  1.00 14.91    B   O
ATOM  2068  N   SER B  8    10.444  84.670  47.953  1.00 13.64    B   N
ATOM  2069  CA  SER B  8    11.367  83.551  48.076  1.00 13.32    B   C
ATOM  2070  CB  SER B  8    10.870  82.357  47.246  1.00 11.76    B   C
ATOM  2071  OG  SER B  8    10.643  82.716  45.892  1.00 12.59    B   O
ATOM  2072  C   SER B  8    12.760  83.979  47.618  1.00 12.86    B   C
ATOM  2073  O   SER B  8    13.760  83.328  47.931  1.00 15.56    B   O
ATOM  2074  N   GLY B  9    12.826  85.088  46.888  1.00 14.15    B   N
ATOM  2075  CA  GLY B  9    14.113  85.565  46.418  1.00 11.94    B   C
ATOM  2076  C   GLY B  9    14.060  86.923  45.751  1.00 13.28    B   C
ATOM  2077  O   GLY B  9    13.420  87.855  46.255  1.00 11.42    B   O
ATOM  2078  N   VAL B 10    14.731  87.031  44.608  1.00 11.70    B   N
ATOM  2079  CA  VAL B 10    14.793  88.283  43.848  1.00 13.19    B   C
ATOM  2080  CB  VAL B 10    16.035  88.301  42.931  1.00 11.94    B   C
ATOM  2081  CG1 VAL B 10    15.956  87.149  41.948  1.00 17.01    B   C
ATOM  2082  CG2 VAL B 10    16.148  89.633  42.200  1.00 12.63    B   C
ATOM  2083  C   VAL B 10    13.546  88.495  42.995  1.00 12.34    B   C
ATOM  2084  O   VAL B 10    13.267  89.604  42.550  1.00 14.01    B   O
ATOM  2085  N   GLY B 11    12.794  87.426  42.768  1.00 12.08    B   N
ATOM  2086  CA  GLY B 11    11.591  87.540  41.957  1.00 14.90    B   C
ATOM  2087  C   GLY B 11    10.634  88.640  42.373  1.00 12.77    B   C
ATOM  2088  O   GLY B 11    10.004  89.278  41.524  1.00 13.23    B   O
ATOM  2089  N   GLY B 12    10.524  88.861  43.679  1.00 13.56    B   N
ATOM  2090  CA  GLY B 12     9.639  89.887  44.198  1.00 15.76    B   C
ATOM  2091  C   GLY B 12     9.917  91.279  43.659  1.00 15.26    B   C
ATOM  2092  O   GLY B 12     9.141  92.213  43.899  1.00 15.12    B   O
ATOM  2093  N   PHE B 13    11.024  91.426  42.937  1.00 12.59    B   N
ATOM  2094  CA  PHE B 13    11.376  92.713  42.360  1.00 14.03    B   C
ATOM  2095  CB  PHE B 13    12.702  92.620  41.589  1.00 14.04    B   C
ATOM  2096  CG  PHE B 13    13.929  92.823  42.446  1.00 14.87    B   C
ATOM  2097  CD1 PHE B 13    15.133  93.231  41.868  1.00 16.32    B   C
ATOM  2098  CD2 PHE B 13    13.883  92.629  43.823  1.00 14.64    B   C
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Figure 5LL

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ATOM  2099 CE1 PHE B 13     16.272  93.448  42.651  1.00 13.70    B   C
ATOM  2100 CE2 PHE B 13     15.013  92.842  44.614  1.00 13.54    B   C
ATOM  2101 CZ  PHE B 13     16.210  93.254  44.025  1.00 15.35    B   C
ATOM  2102 C   PHE B 13     10.260  93.184  41.425  1.00 14.72    B   C
ATOM  2103 O   PHE B 13     10.013  94.380  41.301  1.00 12.42    B   O
ATOM  2104 N   SER B 14      9.580  92.243  40.775  1.00 14.71    B   N
ATOM  2105 CA  SER B 14      8.494  92.600  39.860  1.00 14.65    B   C
ATOM  2106 CB  SER B 14      7.918  91.349  39.187  1.00 14.09    B   C
ATOM  2107 OG  SER B 14      7.405  90.436  40.135  1.00 13.06    B   O
ATOM  2108 C   SER B 14      7.380  93.355  40.587  1.00 14.07    B   C
ATOM  2109 O   SER B 14      6.688  94.187  39.994  1.00 13.89    B   O
ATOM  2110 N   VAL B 15      7.212  93.064  41.872  1.00 14.55    B   N
ATOM  2111 CA  VAL B 15      6.196  93.737  42.675  1.00 14.09    B   C
ATOM  2112 CB  VAL B 15      5.675  92.827  43.814  1.00 12.74    B   C
ATOM  2113 CG1 VAL B 15      4.705  93.600  44.698  1.00 13.09    B   C
ATOM  2114 CG2 VAL B 15      4.971  91.604  43.224  1.00 11.77    B   C
ATOM  2115 C   VAL B 15      6.789  95.003  43.283  1.00 14.70    B   C
ATOM  2116 O   VAL B 15      6.145  96.052  43.307  1.00 13.74    B   O
ATOM  2117 N   LEU B 16      8.022  94.903  43.769  1.00 13.69    B   N
ATOM  2118 CA  LEU B 16      8.679  96.048  44.384  1.00 14.26    B   C
ATOM  2119 CB  LEU B 16     10.082  95.662  44.863  1.00 13.66    B   C
ATOM  2120 CG  LEU B 16     10.940  96.793  45.448  1.00 14.21    B   C
ATOM  2121 CD1 LEU B 16     10.201  97.451  46.605  1.00 12.59    B   C
ATOM  2122 CD2 LEU B 16     12.280  96.242  45.905  1.00 12.19    B   C
ATOM  2123 C   LEU B 16      8.757  97.212  43.401  1.00 16.29    B   C
ATOM  2124 O   LEU B 16      8.614  98.373  43.787  1.00 16.57    B   O
ATOM  2125 N   LYS B 17      8.984  96.896  42.129  1.00 17.51    B   N
ATOM  2126 CA  LYS B 17      9.069  97.927  41.099  1.00 19.45    B   C
ATOM  2127 CB  LYS B 17      9.349  97.298  39.733  1.00 19.95    B   C
ATOM  2128 CG  LYS B 17      9.302  98.291  38.578  1.00 24.40    B   C
ATOM  2129 CD  LYS B 17      9.568  97.608  37.245  1.00 29.79    B   C
ATOM  2130 CE  LYS B 17      9.472  98.586  36.081  1.00 33.15    B   C
ATOM  2131 NZ  LYS B 17      9.808  97.925  34.784  1.00 35.04    B   N
ATOM  2132 C   LYS B 17      7.769  98.722  41.038  1.00 19.40    B   C
ATOM  2133 O   LYS B 17      7.788  99.950  40.985  1.00 18.81    B   O
ATOM  2134 N   SER B 18      6.642  98.018  41.042  1.00 18.29    B   N
ATOM  2135 CA  SER B 18      5.344  98.675  40.997  1.00 18.21    B   C
ATOM  2136 CB  SER B 18      4.221  97.636  40.941  1.00 17.21    B   C
ATOM  2137 OG  SER B 18      4.357  96.808  39.798  1.00 17.80    B   O
ATOM  2138 C   SER B 18      5.162  99.561  42.222  1.00 19.88    B   C
ATOM  2139 O   SER B 18      4.720 100.703  42.112  1.00 17.77    B   O
ATOM  2140 N   LEU B 19      5.510  99.030  43.391  1.00 19.41    B   N
ATOM  2141 CA  LEU B 19      5.379  99.785  44.629  1.00 19.33    B   C
ATOM  2142 CB  LEU B 19      5.839  98.936  45.817  1.00 18.90    B   C
ATOM  2143 CG  LEU B 19      5.085  97.622  46.027  1.00 20.11    B   C
ATOM  2144 CD1 LEU B 19      5.701  96.850  47.188  1.00 18.40    B   C
ATOM  2145 CD2 LEU B 19      3.612  97.919  46.289  1.00 17.29    B   C
ATOM  2146 C   LEU B 19      6.205 101.063  44.564  1.00 18.96    B   C
ATOM  2147 O   LEU B 19      5.722 102.145  44.897  1.00 19.77    B   O
ATOM  2148 N   LEU B 20      7.455 100.930  44.136  1.00 19.62    B   N
ATOM  2149 CA  LEU B 20      8.355 102.071  44.024  1.00 20.54    B   C
ATOM  2150 CB  LEU B 20      9.736 101.605  43.548  1.00 19.03    B   C
ATOM  2151 CG  LEU B 20     10.562 100.763  44.529  1.00 21.61    B   C
ATOM  2152 CD1 LEU B 20     11.789 100.217  43.824  1.00 17.66    B   C
ATOM  2153 CD2 LEU B 20     10.968 101.613  45.731  1.00 17.70    B   C
ATOM  2154 C   LEU B 20      7.821 103.148  43.077  1.00 21.80    B   C
ATOM  2155 O   LEU B 20      7.864 104.334  43.397  1.00 24.32    B   O
ATOM  2156 N   LYS B 21      7.321 102.736  41.916  1.00 22.92    B   N
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Figure 5MM

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ATOM  2157  CA  LYS B  21      6.789 103.680  40.932  1.00 25.60      B   C
ATOM  2158  CB  LYS B  21      6.334 102.934  39.671  1.00 29.64      B   C
ATOM  2159  CG  LYS B  21      7.412 102.050  39.049  1.00 39.78      B   C
ATOM  2160  CD  LYS B  21      6.819 100.964  38.139  1.00 45.78      B   C
ATOM  2161  CE  LYS B  21      6.314 101.521  36.813  1.00 49.52      B   C
ATOM  2162  NZ  LYS B  21      7.428 101.970  35.926  1.00 52.40      B   N
ATOM  2163  C   LYS B  21      5.610 104.455  41.513  1.00 24.12      B   C
ATOM  2164  O   LYS B  21      5.461 105.652  41.270  1.00 21.99      B   O
ATOM  2165  N   ALA B  22      4.775 103.762  42.281  1.00 22.32      B   N
ATOM  2166  CA  ALA B  22      3.602 104.378  42.889  1.00 23.02      B   C
ATOM  2167  CB  ALA B  22      2.619 103.299  43.321  1.00 21.51      B   C
ATOM  2168  C   ALA B  22      3.950 105.279  44.074  1.00 25.48      B   C
ATOM  2169  O   ALA B  22      3.082 105.975  44.602  1.00 26.34      B   O
ATOM  2170  N   ARG B  23      5.214 105.264  44.489  1.00 26.06      B   N
ATOM  2171  CA  ARG B  23      5.674 106.090  45.606  1.00 28.97      B   C
ATOM  2172  CB  ARG B  23      5.794 107.556  45.170  1.00 33.33      B   C
ATOM  2173  CG  ARG B  23      6.504 107.770  43.850  1.00 41.37      B   C
ATOM  2174  CD  ARG B  23      6.349 109.205  43.378  1.00 47.44      B   C
ATOM  2175  NE  ARG B  23      6.782 109.366  41.992  1.00 56.48      B   N
ATOM  2176  CZ  ARG B  23      6.602 110.472  41.275  1.00 59.85      B   C
ATOM  2177  NH1 ARG B  23      5.998 111.520  41.819  1.00 63.01      B   N
ATOM  2178  NH2 ARG B  23      7.019 110.529  40.015  1.00 61.13      B   N
ATOM  2179  C   ARG B  23      4.697 106.012  46.774  1.00 27.89      B   C
ATOM  2180  O   ARG B  23      4.246 107.042  47.276  1.00 27.91      B   O
ATOM  2181  N   LEU B  24      4.373 104.797  47.205  1.00 25.94      B   N
ATOM  2182  CA  LEU B  24      3.430 104.611  48.303  1.00 24.48      B   C
ATOM  2183  CB  LEU B  24      2.653 103.301  48.118  1.00 22.57      B   C
ATOM  2184  CG  LEU B  24      1.822 103.103  46.847  1.00 24.84      B   C
ATOM  2185  CD1 LEU B  24      1.067 101.779  46.942  1.00 23.08      B   C
ATOM  2186  CD2 LEU B  24      0.842 104.266  46.671  1.00 23.49      B   C
ATOM  2187  C   LEU B  24      4.048 104.617  49.699  1.00 24.22      B   C
ATOM  2188  O   LEU B  24      3.445 105.126  50.641  1.00 25.35      B   O
ATOM  2189  N   PHE B  25      5.250 104.068  49.842  1.00 25.14      B   N
ATOM  2190  CA  PHE B  25      5.865 103.997  51.161  1.00 25.20      B   C
ATOM  2191  CB  PHE B  25      6.078 102.531  51.530  1.00 24.64      B   C
ATOM  2192  CG  PHE B  25      4.886 101.665  51.251  1.00 23.70      B   C
ATOM  2193  CD1 PHE B  25      4.849 100.851  50.123  1.00 23.04      B   C
ATOM  2194  CD2 PHE B  25      3.788 101.685  52.098  1.00 22.47      B   C
ATOM  2195  CE1 PHE B  25      3.729 100.070  49.845  1.00 20.01      B   C
ATOM  2196  CE2 PHE B  25      2.666 100.910  51.828  1.00 22.66      B   C
ATOM  2197  CZ  PHE B  25      2.637 100.100  50.697  1.00 21.24      B   C
ATOM  2198  C   PHE B  25      7.164 104.758  51.361  1.00 25.96      B   C
ATOM  2199  O   PHE B  25      8.020 104.796  50.482  1.00 28.54      B   O
ATOM  2200  N   ASP B  26      7.308 105.355  52.540  1.00 26.35      B   N
ATOM  2201  CA  ASP B  26      8.512 106.108  52.872  1.00 28.67      B   C
ATOM  2202  CB  ASP B  26      8.300 106.958  54.130  1.00 31.57      B   C
ATOM  2203  CG  ASP B  26      7.335 108.101  53.907  1.00 33.21      B   C
ATOM  2204  OD1 ASP B  26      7.429 108.753  52.844  1.00 33.40      B   O
ATOM  2205  OD2 ASP B  26      6.495 108.352  54.800  1.00 37.72      B   O
ATOM  2206  C   ASP B  26      9.697 105.186  53.109  1.00 25.51      B   C
ATOM  2207  O   ASP B  26     10.840 105.567  52.877  1.00 22.85      B   O
ATOM  2208  N   GLU B  27      9.421 103.974  53.581  1.00 24.08      B   N
ATOM  2209  CA  GLU B  27     10.483 103.013  53.859  1.00 21.60      B   C
ATOM  2210  CB  GLU B  27     10.964 103.179  55.305  1.00 22.98      B   C
ATOM  2211  CG  GLU B  27     11.869 102.071  55.800  1.00 25.73      B   C
ATOM  2212  CD  GLU B  27     12.636 102.459  57.051  1.00 30.40      B   C
ATOM  2213  OE1 GLU B  27     12.088 103.219  57.883  1.00 28.18      B   O
ATOM  2214  OE2 GLU B  27     13.785 101.993  57.207  1.00 28.75      B   O
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Figure 5NN

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ATOM  2215  C  GLU B  27     10.036 101.576  53.601  1.00 19.70    B   C
ATOM  2216  O  GLU B  27      8.919 101.184  53.948  1.00 17.68    B   O
ATOM  2217  N  ILE B  28     10.926 100.795  52.995  1.00 16.91    B   N
ATOM  2218  CA ILE B  28     10.630  99.407  52.651  1.00 14.07    B   C
ATOM  2219  CB ILE B  28     10.394  99.276  51.121  1.00 15.11    B   C
ATOM  2220  CG2 ILE B  28     10.279  97.816  50.711  1.00 15.06    B   C
ATOM  2221  CG1 ILE B  28      9.124 100.034  50.732  1.00 15.08    B   C
ATOM  2222  CD1 ILE B  28      8.920 100.162  49.218  1.00 17.55    B   C
ATOM  2223  C  ILE B  28     11.740  98.446  53.069  1.00 14.73    B   C
ATOM  2224  O  ILE B  28     12.925  98.694  52.825  1.00 14.43    B   O
ATOM  2225  N  ILE B  29     11.348  97.357  53.720  1.00 13.73    B   N
ATOM  2226  CA ILE B  29     12.299  96.338  54.143  1.00 15.11    B   C
ATOM  2227  CB ILE B  29     12.113  95.957  55.636  1.00 14.64    B   C
ATOM  2228  CG2 ILE B  29     13.231  95.012  56.077  1.00 13.07    B   C
ATOM  2229  CG1 ILE B  29     12.129  97.214  56.521  1.00 16.50    B   C
ATOM  2230  CD1 ILE B  29     13.462  97.949  56.554  1.00 12.57    B   C
ATOM  2231  C  ILE B  29     11.989  95.121  53.262  1.00 14.26    B   C
ATOM  2232  O  ILE B  29     10.960  94.460  53.438  1.00 16.06    B   O
ATOM  2233  N  TYR B  30     12.857  94.855  52.293  1.00 12.97    B   N
ATOM  2234  CA TYR B  30     12.667  93.728  51.382  1.00 12.66    B   C
ATOM  2235  CB TYR B  30     13.095  94.117  49.957  1.00 11.95    B   C
ATOM  2236  CG TYR B  30     12.831  93.042  48.913  1.00 11.71    B   C
ATOM  2237  CD1 TYR B  30     11.703  93.097  48.096  1.00  9.69    B   C
ATOM  2238  CE1 TYR B  30     11.441  92.100  47.149  1.00 12.54    B   C
ATOM  2239  CD2 TYR B  30     13.700  91.958  48.762  1.00 12.15    B   C
ATOM  2240  CE2 TYR B  30     13.449  90.953  47.817  1.00 14.27    B   C
ATOM  2241  CZ  TYR B  30     12.319  91.033  47.014  1.00 14.57    B   C
ATOM  2242  OH  TYR B  30     12.078  90.061  46.070  1.00 11.66    B   O
ATOM  2243  C  TYR B  30     13.473  92.516  51.842  1.00 15.13    B   C
ATOM  2244  O  TYR B  30     14.673  92.624  52.115  1.00 17.82    B   O
ATOM  2245  N  TYR B  31     12.812  91.364  51.932  1.00 13.53    B   N
ATOM  2246  CA TYR B  31     13.488  90.144  52.350  1.00 13.30    B   C
ATOM  2247  CB TYR B  31     13.063  89.742  53.773  1.00 14.35    B   C
ATOM  2248  CG TYR B  31     13.588  88.381  54.209  1.00 13.93    B   C
ATOM  2249  CD1 TYR B  31     14.955  88.143  54.318  1.00 13.81    B   C
ATOM  2250  CE1 TYR B  31     15.446  86.887  54.682  1.00 16.52    B   C
ATOM  2251  CD2 TYR B  31     12.712  87.326  54.481  1.00 15.49    B   C
ATOM  2252  CE2 TYR B  31     13.191  86.064  54.850  1.00 17.62    B   C
ATOM  2253  CZ  TYR B  31     14.563  85.852  54.946  1.00 14.49    B   C
ATOM  2254  OH  TYR B  31     15.047  84.611  55.304  1.00 14.75    B   O
ATOM  2255  C  TYR B  31     13.188  89.005  51.382  1.00 11.69    B   C
ATOM  2256  O  TYR B  31     12.032  88.657  51.153  1.00 12.79    B   O
ATOM  2257  N  GLY B  32     14.246  88.440  50.812  1.00 12.78    B   N
ATOM  2258  CA GLY B  32     14.093  87.327  49.896  1.00 11.28    B   C
ATOM  2259  C  GLY B  32     14.761  86.117  50.522  1.00 13.78    B   C
ATOM  2260  O  GLY B  32     15.950  86.162  50.839  1.00 11.17    B   O
ATOM  2261  N  ASP B  33     14.002  85.040  50.710  1.00 14.25    B   N
ATOM  2262  CA ASP B  33     14.540  83.819  51.306  1.00 15.29    B   C
ATOM  2263  CB ASP B  33     13.391  82.987  51.885  1.00 13.57    B   C
ATOM  2264  CG ASP B  33     13.871  81.730  52.589  1.00 14.42    B   C
ATOM  2265  OD1 ASP B  33     15.034  81.702  53.046  1.00 14.38    B   O
ATOM  2266  OD2 ASP B  33     13.077  80.773  52.695  1.00 14.44    B   O
ATOM  2267  C  ASP B  33     15.288  83.049  50.226  1.00 14.09    B   C
ATOM  2268  O  ASP B  33     15.027  81.867  49.980  1.00 12.43    B   O
ATOM  2269  N  SER B  34     16.238  83.739  49.597  1.00 14.94    B   N
ATOM  2270  CA SER B  34     17.016  83.186  48.490  1.00 14.92    B   C
ATOM  2271  CB SER B  34     17.941  84.268  47.908  1.00 13.20    B   C
ATOM  2272  OG SER B  34     18.886  84.714  48.863  1.00 14.39    B   O
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Figure 5OO

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ATOM  2273 C   SER B 34    17.821  81.924  48.772  1.00 14.53    B   C
ATOM  2274 O   SER B 34    18.348  81.308  47.849  1.00 12.91    B   O
ATOM  2275 N   ALA B 35    17.930  81.535  50.034  1.00 13.97    B   N
ATOM  2276 CA  ALA B 35    18.664  80.317  50.345  1.00 15.25    B   C
ATOM  2277 CB  ALA B 35    19.050  80.297  51.820  1.00 15.69    B   C
ATOM  2278 C   ALA B 35    17.801  79.101  50.023  1.00 15.43    B   C
ATOM  2279 O   ALA B 35    18.321  78.010  49.776  1.00 13.55    B   O
ATOM  2280 N   ARG B 36    16.484  79.296  50.000  1.00 13.78    B   N
ATOM  2281 CA  ARG B 36    15.567  78.185  49.777  1.00 14.22    B   C
ATOM  2282 CB  ARG B 36    14.697  78.023  51.027  1.00 13.17    B   C
ATOM  2283 CG  ARG B 36    15.541  77.986  52.303  1.00 13.84    B   C
ATOM  2284 CD  ARG B 36    14.775  77.513  53.520  1.00 16.20    B   C
ATOM  2285 NE  ARG B 36    13.830  78.511  54.012  1.00 13.15    B   N
ATOM  2286 CZ  ARG B 36    13.310  78.500  55.235  1.00 14.54    B   C
ATOM  2287 NH1 ARG B 36    13.642  77.542  56.090  1.00 13.26    B   N
ATOM  2288 NH2 ARG B 36    12.468  79.454  55.613  1.00 15.47    B   N
ATOM  2289 C   ARG B 36    14.703  78.235  48.517  1.00 14.96    B   C
ATOM  2290 O   ARG B 36    13.971  77.288  48.220  1.00 16.93    B   O
ATOM  2291 N   VAL B 37    14.791  79.328  47.770  1.00 14.56    B   N
ATOM  2292 CA  VAL B 37    14.036  79.461  46.530  1.00 15.83    B   C
ATOM  2293 CB  VAL B 37    14.327  80.840  45.875  1.00 16.33    B   C
ATOM  2294 CG1 VAL B 37    15.775  80.909  45.422  1.00 16.98    B   C
ATOM  2295 CG2 VAL B 37    13.379  81.093  44.719  1.00 16.47    B   C
ATOM  2296 C   VAL B 37    14.452  78.312  45.587  1.00 14.68    B   C
ATOM  2297 O   VAL B 37    15.615  77.895  45.575  1.00 15.45    B   O
ATOM  2298 N   PRO B 38    13.511  77.780  44.790  1.00 14.64    B   N
ATOM  2299 CD  PRO B 38    13.845  76.783  43.755  1.00 11.60    B   C
ATOM  2300 CA  PRO B 38    12.102  78.160  44.696  1.00 14.93    B   C
ATOM  2301 CB  PRO B 38    11.743  77.754  43.271  1.00 13.51    B   C
ATOM  2302 CG  PRO B 38    12.485  76.470  43.123  1.00 15.17    B   C
ATOM  2303 C   PRO B 38    11.191  77.489  45.710  1.00 15.27    B   C
ATOM  2304 O   PRO B 38    11.510  76.437  46.274  1.00 13.54    B   O
ATOM  2305 N   TYR B 39    10.043  78.118  45.915  1.00 13.69    B   N
ATOM  2306 CA  TYR B 39     9.013  77.623  46.811  1.00 13.90    B   C
ATOM  2307 CB  TYR B 39     8.268  78.798  47.444  1.00 13.72    B   C
ATOM  2308 CG  TYR B 39     8.922  79.471  48.624  1.00 10.70    B   C
ATOM  2309 CD1 TYR B 39    10.268  79.261  48.937  1.00 10.84    B   C
ATOM  2310 CE1 TYR B 39    10.860  79.906  50.023  1.00 12.25    B   C
ATOM  2311 CD2 TYR B 39     8.186  80.344  49.426  1.00 12.79    B   C
ATOM  2312 CE2 TYR B 39     8.766  80.996  50.514  1.00 12.39    B   C
ATOM  2313 CZ  TYR B 39    10.104  80.772  50.809  1.00 13.35    B   C
ATOM  2314 OH  TYR B 39    10.674  81.405  51.893  1.00 12.01    B   O
ATOM  2315 C   TYR B 39     7.997  76.821  45.987  1.00 14.02    B   C
ATOM  2316 O   TYR B 39     7.451  75.827  46.455  1.00 15.23    B   O
ATOM  2317 N   GLY B 40     7.752  77.290  44.765  1.00 16.75    B   N
ATOM  2318 CA  GLY B 40     6.768  76.686  43.874  1.00 16.84    B   C
ATOM  2319 C   GLY B 40     6.860  75.212  43.525  1.00 16.65    B   C
ATOM  2320 O   GLY B 40     5.886  74.620  43.049  1.00 14.08    B   O
ATOM  2321 N   THR B 41     8.017  74.611  43.766  1.00 15.91    B   N
ATOM  2322 CA  THR B 41     8.225  73.204  43.440  1.00 16.59    B   C
ATOM  2323 CB  THR B 41     9.636  72.990  42.900  1.00 16.07    B   C
ATOM  2324 OG1 THR B 41    10.580  73.477  43.861  1.00 15.88    B   O
ATOM  2325 CG2 THR B 41     9.817  73.737  41.592  1.00 19.86    B   C
ATOM  2326 C   THR B 41     8.072  72.320  44.659  1.00 16.87    B   C
ATOM  2327 O   THR B 41     8.245  71.099  44.584  1.00 18.68    B   O
ATOM  2328 N   LYS B 42     7.742  72.939  45.783  1.00 16.57    B   N
ATOM  2329 CA  LYS B 42     7.647  72.178  47.002  1.00 16.66    B   C
ATOM  2330 CB  LYS B 42     8.592  72.768  48.035  1.00 15.39    B   C
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Figure 5PP

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ATOM  2331  CG  LYS B  42      10.049  72.613  47.578  1.00 16.40      B   C
ATOM  2332  CD  LYS B  42      10.942  73.766  47.995  1.00 12.99      B   C
ATOM  2333  CE  LYS B  42      12.343  73.611  47.372  1.00 12.98      B   C
ATOM  2334  NZ  LYS B  42      13.246  74.754  47.688  1.00 12.01      B   N
ATOM  2335  C   LYS B  42       6.273  71.981  47.593  1.00 19.30      B   C
ATOM  2336  O   LYS B  42       5.311  72.659  47.234  1.00 19.46      B   O
ATOM  2337  N   ASP B  43       6.206  71.042  48.526  1.00 19.11      B   N
ATOM  2338  CA  ASP B  43       4.903  70.766  49.089  1.00 20.39      B   C
ATOM  2339  CB  ASP B  43       4.970  69.389  49.727  1.00 26.23      B   C
ATOM  2340  CG  ASP B  43       3.668  68.908  50.218  1.00 34.18      B   C
ATOM  2341  OD1 ASP B  43       3.032  69.628  51.023  1.00 35.73      B   O
ATOM  2342  OD2 ASP B  43       3.286  67.802  49.834  1.00 34.67      B   O
ATOM  2343  C   ASP B  43       4.324  71.860  50.037  1.00 18.74      B   C
ATOM  2344  O   ASP B  43       5.067  72.590  50.662  1.00 17.52      B   O
ATOM  2345  N   PRO B  44       2.970  71.973  50.139  1.00 16.86      B   N
ATOM  2346  CD  PRO B  44       1.945  71.249  49.366  1.00 16.70      B   C
ATOM  2347  CA  PRO B  44       2.316  72.976  51.001  1.00 15.67      B   C
ATOM  2348  CB  PRO B  44       0.838  72.608  50.910  1.00 16.57      B   C
ATOM  2349  CG  PRO B  44       0.714  72.164  49.520  1.00 15.09      B   C
ATOM  2350  C   PRO B  44       2.785  73.063  52.460  1.00 14.32      B   C
ATOM  2351  O   PRO B  44       2.975  74.159  52.984  1.00 14.18      B   O
ATOM  2352  N   THR B  45       2.968  71.928  53.125  1.00 12.56      B   N
ATOM  2353  CA  THR B  45       3.404  71.976  54.513  1.00 15.07      B   C
ATOM  2354  CB  THR B  45       3.416  70.544  55.159  1.00 14.56      B   C
ATOM  2355  OG1 THR B  45       3.473  70.671  56.582  1.00 20.74      B   O
ATOM  2356  CG2 THR B  45       4.617  69.725  54.690  1.00 16.79      B   C
ATOM  2357  C   THR B  45       4.773  72.673  54.661  1.00 13.75      B   C
ATOM  2358  O   THR B  45       5.015  73.370  55.644  1.00 15.18      B   O
ATOM  2359  N   THR B  46       5.652  72.512  53.675  1.00 14.31      B   N
ATOM  2360  CA  THR B  46       6.978  73.138  53.708  1.00 13.76      B   C
ATOM  2361  CB  THR B  46       7.908  72.534  52.625  1.00 15.70      B   C
ATOM  2362  OG1 THR B  46       8.111  71.139  52.888  1.00 16.08      B   O
ATOM  2363  CG2 THR B  46       9.257  73.237  52.611  1.00 14.55      B   C
ATOM  2364  C   THR B  46       6.874  74.645  53.463  1.00 14.40      B   C
ATOM  2365  O   THR B  46       7.538  75.450  54.120  1.00 12.91      B   O
ATOM  2366  N   ILE B  47       6.029  75.016  52.509  1.00 12.98      B   N
ATOM  2367  CA  ILE B  47       5.843  76.414  52.159  1.00 14.06      B   C
ATOM  2368  CB  ILE B  47       4.987  76.537  50.881  1.00 12.60      B   C
ATOM  2369  CG2 ILE B  47       4.790  78.005  50.517  1.00 13.35      B   C
ATOM  2370  CG1 ILE B  47       5.684  75.804  49.727  1.00 14.48      B   C
ATOM  2371  CD1 ILE B  47       4.831  75.660  48.469  1.00 13.95      B   C
ATOM  2372  C   ILE B  47       5.193  77.190  53.305  1.00 13.29      B   C
ATOM  2373  O   ILE B  47       5.588  78.314  53.610  1.00 12.68      B   O
ATOM  2374  N   LYS B  48       4.199  76.594  53.948  1.00 13.12      B   N
ATOM  2375  CA  LYS B  48       3.541  77.279  55.047  1.00 14.82      B   C
ATOM  2376  CB  LYS B  48       2.387  76.440  55.606  1.00 15.61      B   C
ATOM  2377  CG  LYS B  48       1.239  76.283  54.621  1.00 16.82      B   C
ATOM  2378  CD  LYS B  48       0.021  75.649  55.261  1.00 17.71      B   C
ATOM  2379  CE  LYS B  48      -1.123  75.558  54.259  1.00 21.58      B   C
ATOM  2380  NZ  LYS B  48      -2.370  75.047  54.891  1.00 23.95      B   N
ATOM  2381  C   LYS B  48       4.537  77.600  56.145  1.00 15.64      B   C
ATOM  2382  O   LYS B  48       4.546  78.719  56.661  1.00 14.41      B   O
ATOM  2383  N   GLN B  49       5.383  76.630  56.493  1.00 13.94      B   N
ATOM  2384  CA  GLN B  49       6.388  76.836  57.533  1.00 14.63      B   C
ATOM  2385  CB  GLN B  49       7.127  75.520  57.822  1.00 15.57      B   C
ATOM  2386  CG  GLN B  49       8.185  75.577  58.930  1.00 19.33      B   C
ATOM  2387  CD  GLN B  49       7.656  76.099  60.258  1.00 18.82      B   C
ATOM  2388  OE1 GLN B  49       6.509  75.840  60.638  1.00 17.48      B   O
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Figure 5QQ

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ATOM  2389 NE2 GLN B 49     8.498 76.826 60.977 1.00 19.58    B   N
ATOM  2390 C   GLN B 49     7.357 77.934 57.091 1.00 15.00    B   C
ATOM  2391 O   GLN B 49     7.754 78.773 57.898 1.00 15.49    B   O
ATOM  2392 N   PHE B 50     7.732 77.936 55.812 1.00 13.73    B   N
ATOM  2393 CA  PHE B 50     8.617 78.978 55.297 1.00 12.73    B   C
ATOM  2394 CB  PHE B 50     8.813 78.845 53.784 1.00 12.69    B   C
ATOM  2395 CG  PHE B 50     9.756 77.740 53.372 1.00 14.11    B   C
ATOM  2396 CD1 PHE B 50    10.540 77.073 54.310 1.00 13.47    B   C
ATOM  2397 CD2 PHE B 50     9.884 77.396 52.028 1.00 16.97    B   C
ATOM  2398 CE1 PHE B 50    11.442 76.080 53.915 1.00 14.96    B   C
ATOM  2399 CE2 PHE B 50    10.784 76.405 51.622 1.00 16.26    B   C
ATOM  2400 CZ  PHE B 50    11.563 75.747 52.569 1.00 13.12    B   C
ATOM  2401 C   PHE B 50     7.999 80.348 55.586 1.00 12.88    B   C
ATOM  2402 O   PHE B 50     8.690 81.281 55.998 1.00 14.04    B   O
ATOM  2403 N   GLY B 51     6.692 80.460 55.353 1.00 13.99    B   N
ATOM  2404 CA  GLY B 51     5.992 81.712 55.590 1.00 13.72    B   C
ATOM  2405 C   GLY B 51     6.023 82.158 57.043 1.00 14.83    B   C
ATOM  2406 O   GLY B 51     6.243 83.334 57.331 1.00 11.98    B   O
ATOM  2407 N   LEU B 52     5.788 81.227 57.966 1.00 15.32    B   N
ATOM  2408 CA  LEU B 52     5.815 81.555 59.388 1.00 18.38    B   C
ATOM  2409 CB  LEU B 52     5.525 80.320 60.248 1.00 18.53    B   C
ATOM  2410 CG  LEU B 52     4.074 79.939 60.511 1.00 24.25    B   C
ATOM  2411 CD1 LEU B 52     3.349 79.724 59.198 1.00 27.80    B   C
ATOM  2412 CD2 LEU B 52     4.037 78.679 61.371 1.00 26.46    B   C
ATOM  2413 C   LEU B 52     7.184 82.091 59.757 1.00 18.61    B   C
ATOM  2414 O   LEU B 52     7.303 83.096 60.455 1.00 21.72    B   O
ATOM  2415 N   GLU B 53     8.219 81.404 59.289 1.00 18.50    B   N
ATOM  2416 CA  GLU B 53     9.584 81.811 59.573 1.00 17.94    B   C
ATOM  2417 CB  GLU B 53    10.551 80.751 59.038 1.00 17.42    B   C
ATOM  2418 CG  GLU B 53    10.566 79.507 59.927 1.00 15.49    B   C
ATOM  2419 CD  GLU B 53    11.305 78.332 59.323 1.00 17.96    B   C
ATOM  2420 OE1 GLU B 53    12.087 78.534 58.374 1.00 18.58    B   O
ATOM  2421 OE2 GLU B 53    11.105 77.201 59.813 1.00 19.70    B   O
ATOM  2422 C   GLU B 53     9.897 83.193 59.005 1.00 18.71    B   C
ATOM  2423 O   GLU B 53    10.680 83.945 59.579 1.00 19.86    B   O
ATOM  2424 N   ALA B 54     9.271 83.537 57.885 1.00 18.53    B   N
ATOM  2425 CA  ALA B 54     9.492 84.848 57.283 1.00 16.14    B   C
ATOM  2426 CB  ALA B 54     8.744 84.951 55.954 1.00 13.28    B   C
ATOM  2427 C   ALA B 54     9.009 85.934 58.257 1.00 18.34    B   C
ATOM  2428 O   ALA B 54     9.636 86.987 58.393 1.00 16.94    B   O
ATOM  2429 N   LEU B 55     7.898 85.669 58.941 1.00 17.14    B   N
ATOM  2430 CA  LEU B 55     7.361 86.629 59.901 1.00 18.57    B   C
ATOM  2431 CB  LEU B 55     6.118 86.060 60.594 1.00 19.89    B   C
ATOM  2432 CG  LEU B 55     4.827 85.855 59.795 1.00 20.72    B   C
ATOM  2433 CD1 LEU B 55     3.771 85.221 60.706 1.00 22.99    B   C
ATOM  2434 CD2 LEU B 55     4.321 87.192 59.251 1.00 23.42    B   C
ATOM  2435 C   LEU B 55     8.405 86.999 60.956 1.00 18.71    B   C
ATOM  2436 O   LEU B 55     8.555 88.170 61.301 1.00 17.21    B   O
ATOM  2437 N   ASP B 56     9.131 86.002 61.458 1.00 18.83    B   N
ATOM  2438 CA  ASP B 56    10.151 86.241 62.474 1.00 18.36    B   C
ATOM  2439 CB  ASP B 56    10.829 84.924 62.881 1.00 21.45    B   C
ATOM  2440 CG  ASP B 56     9.875 83.958 63.581 1.00 24.57    B   C
ATOM  2441 OD1 ASP B 56     9.003 84.419 64.344 1.00 27.38    B   O
ATOM  2442 OD2 ASP B 56    10.005 82.729 63.383 1.00 26.87    B   O
ATOM  2443 C   ASP B 56    11.211 87.240 62.014 1.00 19.11    B   C
ATOM  2444 O   ASP B 56    11.669 88.082 62.792 1.00 17.72    B   O
ATOM  2445 N   PHE B 57    11.598 87.154 60.746 1.00 17.66    B   N
ATOM  2446 CA  PHE B 57    12.607 88.063 60.216 1.00 16.52    B   C
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Figure 5RR

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ATOM  2447 CB  PHE B  57     12.867  87.794  58.732  1.00 16.73      B   C
ATOM  2448 CG  PHE B  57     13.656  88.879  58.071  1.00 17.10      B   C
ATOM  2449 CD1 PHE B  57     15.035  88.958  58.247  1.00 19.76      B   C
ATOM  2450 CD2 PHE B  57     13.010  89.889  57.366  1.00 14.93      B   C
ATOM  2451 CE1 PHE B  57     15.759  90.031  57.738  1.00 19.78      B   C
ATOM  2452 CE2 PHE B  57     13.721  90.966  56.854  1.00 19.53      B   C
ATOM  2453 CZ  PHE B  57     15.100  91.039  57.041  1.00 19.60      B   C
ATOM  2454 C   PHE B  57     12.222  89.529  60.360  1.00 16.52      B   C
ATOM  2455 O   PHE B  57     13.057  90.365  60.699  1.00 18.03      B   O
ATOM  2456 N   PHE B  58     10.962  89.842  60.082  1.00 15.91      B   N
ATOM  2457 CA  PHE B  58     10.497  91.222  60.144  1.00 18.80      B   C
ATOM  2458 CB  PHE B  58      9.233  91.385  59.295  1.00 17.22      B   C
ATOM  2459 CG  PHE B  58      9.465  91.219  57.825  1.00 18.15      B   C
ATOM  2460 CD1 PHE B  58      9.217  90.004  57.199  1.00 18.00      B   C
ATOM  2461 CD2 PHE B  58      9.927  92.283  57.061  1.00 17.52      B   C
ATOM  2462 CE1 PHE B  58      9.423  89.852  55.831  1.00 16.31      B   C
ATOM  2463 CE2 PHE B  58     10.136  92.142  55.694  1.00 16.57      B   C
ATOM  2464 CZ  PHE B  58      9.884  90.924  55.077  1.00 17.04      B   C
ATOM  2465 C   PHE B  58     10.224  91.809  61.522  1.00 18.66      B   C
ATOM  2466 O   PHE B  58     10.140  93.028  61.662  1.00 21.14      B   O
ATOM  2467 N   LYS B  59     10.080  90.958  62.531  1.00 19.45      B   N
ATOM  2468 CA  LYS B  59      9.769  91.429  63.877  1.00 21.34      B   C
ATOM  2469 CB  LYS B  59      9.816  90.258  64.858  1.00 22.87      B   C
ATOM  2470 CG  LYS B  59      8.740  89.213  64.571  1.00 27.48      B   C
ATOM  2471 CD  LYS B  59      8.762  88.088  65.585  1.00 28.84      B   C
ATOM  2472 CE  LYS B  59      7.612  87.121  65.345  1.00 32.72      B   C
ATOM  2473 NZ  LYS B  59      6.308  87.829  65.430  1.00 35.68      B   N
ATOM  2474 C   LYS B  59     10.614  92.596  64.384  1.00 20.43      B   C
ATOM  2475 O   LYS B  59     10.073  93.621  64.792  1.00 19.96      B   O
ATOM  2476 N   PRO B  60     11.948  92.468  64.356  1.00 20.32      B   N
ATOM  2477 CD  PRO B  60     12.784  91.337  63.911  1.00 19.12      B   C
ATOM  2478 CA  PRO B  60     12.776  93.579  64.837  1.00 19.99      B   C
ATOM  2479 CB  PRO B  60     14.181  92.980  64.848  1.00 21.24      B   C
ATOM  2480 CG  PRO B  60     14.131  91.991  63.719  1.00 22.69      B   C
ATOM  2481 C   PRO B  60     12.690  94.859  63.995  1.00 20.53      B   C
ATOM  2482 O   PRO B  60     13.030  95.943  64.472  1.00 18.48      B   O
ATOM  2483 N   HIS B  61     12.221  94.740  62.756  1.00 18.92      B   N
ATOM  2484 CA  HIS B  61     12.116  95.896  61.871  1.00 20.35      B   C
ATOM  2485 CB  HIS B  61     12.099  95.433  60.413  1.00 19.99      B   C
ATOM  2486 CG  HIS B  61     13.409  94.875  59.953  1.00 19.89      B   C
ATOM  2487 CD2 HIS B  61     13.820  93.599  59.768  1.00 21.62      B   C
ATOM  2488 ND1 HIS B  61     14.499  95.673  59.678  1.00 21.05      B   N
ATOM  2489 CE1 HIS B  61     15.526  94.912  59.343  1.00 22.27      B   C
ATOM  2490 NE2 HIS B  61     15.142  93.649  59.390  1.00 21.05      B   N
ATOM  2491 C   HIS B  61     10.904  96.770  62.170  1.00 21.73      B   C
ATOM  2492 O   HIS B  61     10.808  97.899  61.691  1.00 22.05      B   O
ATOM  2493 N   GLU B  62      9.985  96.242  62.969  1.00 21.87      B   N
ATOM  2494 CA  GLU B  62      8.792  96.982  63.354  1.00 23.56      B   C
ATOM  2495 CB  GLU B  62      9.181  98.106  64.318  1.00 24.92      B   C
ATOM  2496 CG  GLU B  62     10.003  97.606  65.496  1.00 30.01      B   C
ATOM  2497 CD  GLU B  62     10.361  98.699  66.481  1.00 33.69      B   C
ATOM  2498 OE1 GLU B  62     10.896  99.743  66.053  1.00 35.60      B   O
ATOM  2499 OE2 GLU B  62     10.116  98.505  67.688  1.00 36.17      B   O
ATOM  2500 C   GLU B  62      8.044  97.552  62.157  1.00 22.92      B   C
ATOM  2501 O   GLU B  62      7.701  98.739  62.126  1.00 21.97      B   O
ATOM  2502 N   ILE B  63      7.795  96.706  61.164  1.00 19.69      B   N
ATOM  2503 CA  ILE B  63      7.064  97.144  59.987  1.00 18.17      B   C
ATOM  2504 CB  ILE B  63      7.236  96.149  58.825  1.00 17.22      B   C
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Figure 5SS

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ATOM  2505 CG2 ILE B  63      8.686  96.146  58.370  1.00 15.56    B   C
ATOM  2506 CG1 ILE B  63      6.817  94.746  59.269  1.00 15.21    B   C
ATOM  2507 CD1 ILE B  63      6.745  93.736  58.131  1.00 15.19    B   C
ATOM  2508 C   ILE B  63      5.590  97.258  60.375  1.00 18.21    B   C
ATOM  2509 O   ILE B  63      5.127  96.575  61.294  1.00 17.53    B   O
ATOM  2510 N   GLU B  64      4.859  98.125  59.683  1.00 16.97    B   N
ATOM  2511 CA  GLU B  64      3.445  98.349  59.985  1.00 17.61    B   C
ATOM  2512 CB  GLU B  64      3.089  99.813  59.718  1.00 18.92    B   C
ATOM  2513 CG  GLU B  64      3.934 100.801  60.499  1.00 23.07    B   C
ATOM  2514 CD  GLU B  64      3.697 102.235  60.067  1.00 26.42    B   C
ATOM  2515 OE1 GLU B  64      2.541 102.702  60.167  1.00 28.70    B   O
ATOM  2516 OE2 GLU B  64      4.667 102.889  59.624  1.00 25.35    B   O
ATOM  2517 C   GLU B  64      2.511  97.452  59.187  1.00 16.83    B   C
ATOM  2518 O   GLU B  64      1.349  97.259  59.548  1.00 16.07    B   O
ATOM  2519 N   LEU B  65      3.035  96.896  58.104  1.00 17.77    B   N
ATOM  2520 CA  LEU B  65      2.261  96.031  57.232  1.00 16.43    B   C
ATOM  2521 CB  LEU B  65      1.398  96.895  56.302  1.00 18.09    B   C
ATOM  2522 CG  LEU B  65      0.640  96.266  55.133  1.00 21.97    B   C
ATOM  2523 CD1 LEU B  65     -0.529  97.164  54.757  1.00 21.04    B   C
ATOM  2524 CD2 LEU B  65      1.572  96.066  53.944  1.00 20.71    B   C
ATOM  2525 C   LEU B  65      3.244  95.195  56.430  1.00 14.51    B   C
ATOM  2526 O   LEU B  65      4.345  95.648  56.123  1.00 12.92    B   O
ATOM  2527 N   LEU B  66      2.853  93.971  56.102  1.00 14.75    B   N
ATOM  2528 CA  LEU B  66      3.722  93.092  55.329  1.00 14.89    B   C
ATOM  2529 CB  LEU B  66      4.020  91.810  56.110  1.00 14.10    B   C
ATOM  2530 CG  LEU B  66      4.753  90.716  55.326  1.00 16.87    B   C
ATOM  2531 CD1 LEU B  66      6.149  91.214  54.949  1.00 16.67    B   C
ATOM  2532 CD2 LEU B  66      4.844  89.433  56.169  1.00 17.63    B   C
ATOM  2533 C   LEU B  66      3.091  92.722  53.995  1.00 14.55    B   C
ATOM  2534 O   LEU B  66      1.911  92.374  53.923  1.00 16.90    B   O
ATOM  2535 N   ILE B  67      3.884  92.813  52.937  1.00 14.59    B   N
ATOM  2536 CA  ILE B  67      3.422  92.451  51.610  1.00 14.92    B   C
ATOM  2537 CB  ILE B  67      3.775  93.524  50.560  1.00 17.24    B   C
ATOM  2538 CG2 ILE B  67      3.458  93.000  49.150  1.00 14.44    B   C
ATOM  2539 CG1 ILE B  67      2.995  94.815  50.846  1.00 17.41    B   C
ATOM  2540 CD1 ILE B  67      3.287  95.933  49.859  1.00 18.39    B   C
ATOM  2541 C   ILE B  67      4.117  91.159  51.207  1.00 13.22    B   C
ATOM  2542 O   ILE B  67      5.344  91.077  51.219  1.00 13.66    B   O
ATOM  2543 N   VAL B  68      3.330  90.144  50.875  1.00 13.61    B   N
ATOM  2544 CA  VAL B  68      3.898  88.878  50.430  1.00 13.77    B   C
ATOM  2545 CB  VAL B  68      3.065  87.683  50.915  1.00 12.35    B   C
ATOM  2546 CG1 VAL B  68      3.692  86.381  50.426  1.00 10.26    B   C
ATOM  2547 CG2 VAL B  68      2.991  87.699  52.438  1.00 12.86    B   C
ATOM  2548 C   VAL B  68      3.865  88.950  48.907  1.00 12.64    B   C
ATOM  2549 O   VAL B  68      2.839  88.673  48.283  1.00 14.77    B   O
ATOM  2550 N   ALA B  69      4.988  89.349  48.319  1.00 12.26    B   N
ATOM  2551 CA  ALA B  69      5.101  89.499  46.870  1.00 10.06    B   C
ATOM  2552 CB  ALA B  69      6.412  90.194  46.529  1.00  9.84    B   C
ATOM  2553 C   ALA B  69      5.027  88.163  46.147  1.00 12.35    B   C
ATOM  2554 O   ALA B  69      4.635  88.096  44.980  1.00  9.71    B   O
ATOM  2555 N   CYS B  70      5.427  87.104  46.844  1.00 11.11    B   N
ATOM  2556 CA  CYS B  70      5.418  85.766  46.273  1.00 11.24    B   C
ATOM  2557 CB  CYS B  70      6.207  84.816  47.176  1.00 11.62    B   C
ATOM  2558 SG  CYS B  70      6.347  83.142  46.504  1.00 12.64    B   S
ATOM  2559 C   CYS B  70      4.001  85.229  46.070  1.00 11.05    B   C
ATOM  2560 O   CYS B  70      3.205  85.177  47.010  1.00 11.37    B   O
ATOM  2561 N   ASN B  71      3.688  84.823  44.840  1.00 12.49    B   N
ATOM  2562 CA  ASN B  71      2.365  84.279  44.543  1.00 11.50    B   C
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Figure 5TT

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ATOM  2563  CB  ASN B  71      2.157  84.145  43.031  1.00  9.14      B   C
ATOM  2564  CG  ASN B  71      2.258  85.471  42.306  1.00 11.76      B   C
ATOM  2565  OD1 ASN B  71      3.344  86.024  42.151  1.00 10.78      B   O
ATOM  2566  ND2 ASN B  71      1.117  85.996  41.867  1.00 11.54      B   N
ATOM  2567  C   ASN B  71      2.192  82.909  45.186  1.00 12.35      B   C
ATOM  2568  O   ASN B  71      1.078  82.526  45.575  1.00  8.22      B   O
ATOM  2569  N   THR B  72      3.292  82.164  45.270  1.00 11.41      B   N
ATOM  2570  CA  THR B  72      3.257  80.831  45.863  1.00 12.16      B   C
ATOM  2571  CB  THR B  72      4.572  80.062  45.611  1.00 13.52      B   C
ATOM  2572  OG1 THR B  72      4.704  79.791  44.212  1.00 14.69      B   O
ATOM  2573  CG2 THR B  72      4.581  78.741  46.380  1.00 11.87      B   C
ATOM  2574  C   THR B  72      3.012  80.915  47.357  1.00 12.59      B   C
ATOM  2575  O   THR B  72      2.166  80.200  47.892  1.00 14.73      B   O
ATOM  2576  N   ALA B  73      3.754  81.784  48.034  1.00 13.02      B   N
ATOM  2577  CA  ALA B  73      3.576  81.953  49.471  1.00 13.51      B   C
ATOM  2578  CB  ALA B  73      4.676  82.830  50.044  1.00 13.14      B   C
ATOM  2579  C   ALA B  73      2.206  82.571  49.739  1.00 13.74      B   C
ATOM  2580  O   ALA B  73      1.580  82.278  50.752  1.00 12.89      B   O
ATOM  2581  N   SER B  74      1.751  83.437  48.830  1.00 14.66      B   N
ATOM  2582  CA  SER B  74      0.439  84.066  48.967  1.00 14.25      B   C
ATOM  2583  CB  SER B  74      0.212  85.099  47.853  1.00 13.54      B   C
ATOM  2584  OG  SER B  74      0.996  86.268  48.040  1.00 13.45      B   O
ATOM  2585  C   SER B  74     -0.655  83.002  48.877  1.00 16.32      B   C
ATOM  2586  O   SER B  74     -1.668  83.065  49.575  1.00 14.08      B   O
ATOM  2587  N   ALA B  75     -0.443  82.028  48.002  1.00 16.22      B   N
ATOM  2588  CA  ALA B  75     -1.416  80.966  47.797  1.00 17.85      B   C
ATOM  2589  CB  ALA B  75     -1.170  80.291  46.449  1.00 18.98      B   C
ATOM  2590  C   ALA B  75     -1.438  79.911  48.890  1.00 18.56      B   C
ATOM  2591  O   ALA B  75     -2.498  79.377  49.217  1.00 19.22      B   O
ATOM  2592  N   LEU B  76     -0.274  79.608  49.455  1.00 17.86      B   N
ATOM  2593  CA  LEU B  76     -0.196  78.570  50.473  1.00 19.90      B   C
ATOM  2594  CB  LEU B  76      0.921  77.580  50.131  1.00 19.60      B   C
ATOM  2595  CG  LEU B  76      0.703  76.565  49.004  1.00 21.94      B   C
ATOM  2596  CD1 LEU B  76     -0.579  75.764  49.283  1.00 19.11      B   C
ATOM  2597  CD2 LEU B  76      0.610  77.284  47.670  1.00 23.22      B   C
ATOM  2598  C   LEU B  76     -0.021  78.978  51.925  1.00 19.97      B   C
ATOM  2599  O   LEU B  76     -0.643  78.388  52.800  1.00 19.54      B   O
ATOM  2600  N   ALA B  77      0.815  79.980  52.183  1.00 20.55      B   N
ATOM  2601  CA  ALA B  77      1.111  80.380  53.559  1.00 22.00      B   C
ATOM  2602  CB  ALA B  77      2.616  80.581  53.700  1.00 20.40      B   C
ATOM  2603  C   ALA B  77      0.392  81.590  54.149  1.00 21.97      B   C
ATOM  2604  O   ALA B  77      0.420  81.792  55.365  1.00 17.66      B   O
ATOM  2605  N   LEU B  78     -0.247  82.386  53.299  1.00 23.46      B   N
ATOM  2606  CA  LEU B  78     -0.916  83.595  53.757  1.00 24.17      B   C
ATOM  2607  CB  LEU B  78     -1.634  84.271  52.583  1.00 23.46      B   C
ATOM  2608  CG  LEU B  78     -2.166  85.692  52.799  1.00 24.62      B   C
ATOM  2609  CD1 LEU B  78     -1.042  86.612  53.256  1.00 25.18      B   C
ATOM  2610  CD2 LEU B  78     -2.770  86.204  51.499  1.00 21.11      B   C
ATOM  2611  C   LEU B  78     -1.885  83.387  54.918  1.00 23.63      B   C
ATOM  2612  O   LEU B  78     -1.820  84.098  55.918  1.00 20.90      B   O
ATOM  2613  N   GLU B  79     -2.775  82.410  54.798  1.00 24.20      B   N
ATOM  2614  CA  GLU B  79     -3.744  82.171  55.856  1.00 25.27      B   C
ATOM  2615  CB  GLU B  79     -4.643  80.987  55.496  1.00 27.94      B   C
ATOM  2616  CG  GLU B  79     -5.845  80.830  56.417  1.00 34.09      B   C
ATOM  2617  CD  GLU B  79     -6.760  79.694  55.997  1.00 36.98      B   C
ATOM  2618  OE1 GLU B  79     -7.246  79.714  54.847  1.00 38.97      B   O
ATOM  2619  OE2 GLU B  79     -6.994  78.781  56.818  1.00 40.71      B   O
ATOM  2620  C   GLU B  79     -3.066  81.921  57.199  1.00 24.66      B   C
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Figure 5UU

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ATOM  2621  O   GLU B  79     -3.434  82.519  58.208  1.00 21.76      B   O
ATOM  2622  N   GLU B  80     -2.063  81.050  57.213  1.00 25.11      B   N
ATOM  2623  CA  GLU B  80     -1.367  80.740  58.455  1.00 25.16      B   C
ATOM  2624  CB  GLU B  80     -0.425  79.549  58.249  1.00 30.59      B   C
ATOM  2625  CG  GLU B  80     -0.324  78.632  59.464  1.00 36.68      B   C
ATOM  2626  CD  GLU B  80     -1.674  78.055  59.876  1.00 39.61      B   C
ATOM  2627  OE1 GLU B  80     -2.275  77.297  59.085  1.00 42.54      B   O
ATOM  2628  OE2 GLU B  80     -2.139  78.363  60.993  1.00 41.38      B   O
ATOM  2629  C   GLU B  80     -0.587  81.942  58.987  1.00 24.73      B   C
ATOM  2630  O   GLU B  80     -0.590  82.211  60.190  1.00 24.93      B   O
ATOM  2631  N   MET B  81      0.072  82.670  58.092  1.00 22.49      B   N
ATOM  2632  CA  MET B  81      0.851  83.838  58.492  1.00 20.82      B   C
ATOM  2633  CB  MET B  81      1.559  84.437  57.275  1.00 18.38      B   C
ATOM  2634  CG  MET B  81      2.671  83.563  56.717  1.00 18.17      B   C
ATOM  2635  SD  MET B  81      3.255  84.147  55.112  1.00 17.68      B   S
ATOM  2636  CE  MET B  81      4.308  85.481  55.573  1.00 12.45      B   C
ATOM  2637  C   MET B  81     -0.015  84.907  59.155  1.00 20.81      B   C
ATOM  2638  O   MET B  81      0.382  85.508  60.154  1.00 19.23      B   O
ATOM  2639  N   GLN B  82     -1.193  85.145  58.589  1.00 20.82      B   N
ATOM  2640  CA  GLN B  82     -2.111  86.145  59.129  1.00 22.97      B   C
ATOM  2641  CB  GLN B  82     -3.286  86.367  58.168  1.00 23.14      B   C
ATOM  2642  CG  GLN B  82     -2.861  86.867  56.787  1.00 22.68      B   C
ATOM  2643  CD  GLN B  82     -4.024  87.016  55.821  1.00 25.48      B   C
ATOM  2644  OE1 GLN B  82     -4.830  86.097  55.650  1.00 24.87      B   O
ATOM  2645  NE2 GLN B  82     -4.110  88.175  55.172  1.00 25.37      B   N
ATOM  2646  C   GLN B  82     -2.627  85.695  60.482  1.00 22.69      B   C
ATOM  2647  O   GLN B  82     -2.905  86.514  61.357  1.00 22.32      B   O
ATOM  2648  N   LYS B  83     -2.752  84.387  60.656  1.00 24.09      B   N
ATOM  2649  CA  LYS B  83     -3.235  83.851  61.918  1.00 25.60      B   C
ATOM  2650  CB  LYS B  83     -3.376  82.328  61.829  1.00 27.86      B   C
ATOM  2651  CG  LYS B  83     -3.766  81.658  63.141  1.00 32.07      B   C
ATOM  2652  CD  LYS B  83     -3.799  80.148  62.990  1.00 33.64      B   C
ATOM  2653  CE  LYS B  83     -4.118  79.453  64.308  1.00 38.06      B   C
ATOM  2654  NZ  LYS B  83     -4.127  77.965  64.142  1.00 38.15      B   N
ATOM  2655  C   LYS B  83     -2.298  84.218  63.065  1.00 25.66      B   C
ATOM  2656  O   LYS B  83     -2.750  84.586  64.149  1.00 23.94      B   O
ATOM  2657  N   TYR B  84     -0.993  84.134  62.825  1.00 25.08      B   N
ATOM  2658  CA  TYR B  84     -0.022  84.442  63.870  1.00 24.54      B   C
ATOM  2659  CB  TYR B  84      1.063  83.367  63.913  1.00 27.22      B   C
ATOM  2660  CG  TYR B  84      0.542  81.986  64.219  1.00 30.76      B   C
ATOM  2661  CD1 TYR B  84      0.162  81.119  63.195  1.00 31.28      B   C
ATOM  2662  CE1 TYR B  84     -0.325  79.844  63.476  1.00 34.59      B   C
ATOM  2663  CD2 TYR B  84      0.421  81.546  65.538  1.00 32.96      B   C
ATOM  2664  CE2 TYR B  84     -0.066  80.276  65.832  1.00 35.61      B   C
ATOM  2665  CZ  TYR B  84     -0.435  79.430  64.797  1.00 36.06      B   C
ATOM  2666  OH  TYR B  84     -0.904  78.167  65.089  1.00 37.33      B   O
ATOM  2667  C   TYR B  84      0.641  85.808  63.764  1.00 23.89      B   C
ATOM  2668  O   TYR B  84      1.704  86.030  64.341  1.00 25.50      B   O
ATOM  2669  N   SER B  85      0.014  86.726  63.040  1.00 22.10      B   N
ATOM  2670  CA  SER B  85      0.563  88.067  62.874  1.00 21.74      B   C
ATOM  2671  CB  SER B  85      0.884  88.323  61.397  1.00 19.79      B   C
ATOM  2672  OG  SER B  85      1.259  89.673  61.181  1.00 25.60      B   O
ATOM  2673  C   SER B  85     -0.413  89.127  63.374  1.00 21.62      B   C
ATOM  2674  O   SER B  85     -1.621  89.009  63.177  1.00 21.34      B   O
ATOM  2675  N   LYS B  86      0.107  90.157  64.031  1.00 20.33      B   N
ATOM  2676  CA  LYS B  86     -0.750  91.221  64.519  1.00 22.30      B   C
ATOM  2677  CB  LYS B  86     -0.235  91.776  65.853  1.00 25.37      B   C
ATOM  2678  CG  LYS B  86      1.182  92.304  65.826  1.00 31.07      B   C
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Figure 5VV

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ATOM  2679 CD  LYS B 86      1.629  92.685  67.231  1.00 35.40    B   C
ATOM  2680 CE  LYS B 86      1.562  91.486  68.175  1.00 35.66    B   C
ATOM  2681 NZ  LYS B 86      1.952  91.849  69.565  1.00 39.76    B   N
ATOM  2682 C   LYS B 86     -0.860  92.333  63.482  1.00 22.13    B   C
ATOM  2683 O   LYS B 86     -1.871  93.028  63.433  1.00 23.41    B   O
ATOM  2684 N   ILE B 87      0.169  92.499  62.649  1.00 20.24    B   N
ATOM  2685 CA  ILE B 87      0.127  93.524  61.605  1.00 18.31    B   C
ATOM  2686 CB  ILE B 87      1.543  94.004  61.181  1.00 16.92    B   C
ATOM  2687 CG2 ILE B 87      2.244  94.688  62.359  1.00 18.70    B   C
ATOM  2688 CG1 ILE B 87      2.361  92.822  60.650  1.00 17.63    B   C
ATOM  2689 CD1 ILE B 87      3.721  93.203  60.117  1.00 17.00    B   C
ATOM  2690 C   ILE B 87     -0.559  92.921  60.384  1.00 17.72    B   C
ATOM  2691 O   ILE B 87     -0.553  91.707  60.193  1.00 18.08    B   O
ATOM  2692 N   PRO B 88     -1.173  93.762  59.542  1.00 18.77    B   N
ATOM  2693 CD  PRO B 88     -1.340  95.223  59.619  1.00 17.15    B   C
ATOM  2694 CA  PRO B 88     -1.839  93.216  58.358  1.00 19.35    B   C
ATOM  2695 CB  PRO B 88     -2.575  94.428  57.789  1.00 20.10    B   C
ATOM  2696 CG  PRO B 88     -1.691  95.572  58.194  1.00 21.95    B   C
ATOM  2697 C   PRO B 88     -0.844  92.619  57.360  1.00 18.71    B   C
ATOM  2698 O   PRO B 88      0.247  93.148  57.163  1.00 18.85    B   O
ATOM  2699 N   ILE B 89     -1.222  91.498  56.759  1.00 17.91    B   N
ATOM  2700 CA  ILE B 89     -0.387  90.848  55.757  1.00 17.91    B   C
ATOM  2701 CB  ILE B 89     -0.011  89.404  56.164  1.00 18.44    B   C
ATOM  2702 CG2 ILE B 89      0.952  88.807  55.133  1.00 18.14    B   C
ATOM  2703 CG1 ILE B 89      0.658  89.408  57.543  1.00 21.01    B   C
ATOM  2704 CD1 ILE B 89      1.125  88.043  58.007  1.00 18.58    B   C
ATOM  2705 C   ILE B 89     -1.202  90.823  54.466  1.00 17.23    B   C
ATOM  2706 O   ILE B 89     -2.323  90.305  54.425  1.00 17.75    B   O
ATOM  2707 N   VAL B 90     -0.642  91.403  53.414  1.00 16.10    B   N
ATOM  2708 CA  VAL B 90     -1.334  91.467  52.141  1.00 15.66    B   C
ATOM  2709 CB  VAL B 90     -1.436  92.934  51.651  1.00 17.82    B   C
ATOM  2710 CG1 VAL B 90     -2.241  93.001  50.351  1.00 17.58    B   C
ATOM  2711 CG2 VAL B 90     -2.074  93.805  52.739  1.00 18.13    B   C
ATOM  2712 C   VAL B 90     -0.612  90.640  51.088  1.00 13.43    B   C
ATOM  2713 O   VAL B 90      0.567  90.869  50.812  1.00 14.69    B   O
ATOM  2714 N   GLY B 91     -1.332  89.681  50.511  1.00 13.52    B   N
ATOM  2715 CA  GLY B 91     -0.773  88.827  49.474  1.00 12.39    B   C
ATOM  2716 C   GLY B 91     -1.085  89.387  48.093  1.00 14.87    B   C
ATOM  2717 O   GLY B 91     -1.754  90.414  47.982  1.00 13.52    B   O
ATOM  2718 N   VAL B 92     -0.618  88.715  47.041  1.00 13.75    B   N
ATOM  2719 CA  VAL B 92     -0.840  89.190  45.676  1.00 14.98    B   C
ATOM  2720 CB  VAL B 92      0.447  89.066  44.819  1.00 14.03    B   C
ATOM  2721 CG1 VAL B 92      1.442  90.130  45.234  1.00  9.89    B   C
ATOM  2722 CG2 VAL B 92      1.056  87.672  44.978  1.00 12.60    B   C
ATOM  2723 C   VAL B 92     -1.975  88.505  44.922  1.00 16.65    B   C
ATOM  2724 O   VAL B 92     -2.194  88.786  43.746  1.00 17.87    B   O
ATOM  2725 N   ILE B 93     -2.702  87.616  45.585  1.00 16.90    B   N
ATOM  2726 CA  ILE B 93     -3.798  86.933  44.909  1.00 17.60    B   C
ATOM  2727 CB  ILE B 93     -3.993  85.514  45.469  1.00 18.08    B   C
ATOM  2728 CG2 ILE B 93     -5.148  84.825  44.757  1.00 15.25    B   C
ATOM  2729 CG1 ILE B 93     -2.693  84.722  45.291  1.00 18.10    B   C
ATOM  2730 CD1 ILE B 93     -2.803  83.256  45.609  1.00 20.71    B   C
ATOM  2731 C   ILE B 93     -5.125  87.693  44.971  1.00 18.37    B   C
ATOM  2732 O   ILE B 93     -5.720  87.983  43.930  1.00 19.27    B   O
ATOM  2733 N   GLU B 94     -5.590  88.021  46.176  1.00 18.78    B   N
ATOM  2734 CA  GLU B 94     -6.859  88.742  46.315  1.00 21.11    B   C
ATOM  2735 CB  GLU B 94     -7.198  88.977  47.789  1.00 23.95    B   C
ATOM  2736 CG  GLU B 94     -7.565  87.705  48.536  1.00 28.58    B   C
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Figure 5WW

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ATOM  2737 CD  GLU B  94     -8.651  86.906  47.831  1.00 33.34      B   C
ATOM  2738 OE1 GLU B  94     -9.700  87.494  47.484  1.00 32.87      B   O
ATOM  2739 OE2 GLU B  94     -8.453  85.686  47.627  1.00 36.08      B   O
ATOM  2740 C   GLU B  94     -6.873  90.073  45.568  1.00 20.94      B   C
ATOM  2741 O   GLU B  94     -7.882  90.439  44.960  1.00 21.06      B   O
ATOM  2742 N   PRO B  95     -5.760  90.823  45.615  1.00 19.29      B   N
ATOM  2743 CD  PRO B  95     -4.581  90.667  46.487  1.00 17.34      B   C
ATOM  2744 CA  PRO B  95     -5.714  92.108  44.909  1.00 19.84      B   C
ATOM  2745 CB  PRO B  95     -4.301  92.603  45.196  1.00 18.81      B   C
ATOM  2746 CG  PRO B  95     -4.058  92.087  46.580  1.00 19.00      B   C
ATOM  2747 C   PRO B  95     -5.971  91.933  43.415  1.00 18.63      B   C
ATOM  2748 O   PRO B  95     -6.588  92.786  42.771  1.00 19.30      B   O
ATOM  2749 N   SER B  96     -5.485  90.824  42.867  1.00 20.23      B   N
ATOM  2750 CA  SER B  96     -5.661  90.532  41.451  1.00 19.54      B   C
ATOM  2751 CB  SER B  96     -4.752  89.380  41.032  1.00 20.19      B   C
ATOM  2752 OG  SER B  96     -3.398  89.803  41.022  1.00 21.10      B   O
ATOM  2753 C   SER B  96     -7.107  90.194  41.137  1.00 19.82      B   C
ATOM  2754 O   SER B  96     -7.623  90.554  40.076  1.00 18.36      B   O
ATOM  2755 N   ILE B  97     -7.761  89.496  42.060  1.00 19.40      B   N
ATOM  2756 CA  ILE B  97     -9.159  89.129  41.869  1.00 21.46      B   C
ATOM  2757 CB  ILE B  97     -9.702  88.310  43.066  1.00 20.75      B   C
ATOM  2758 CG2 ILE B  97    -11.185  88.032  42.872  1.00 23.74      B   C
ATOM  2759 CG1 ILE B  97     -8.929  86.996  43.205  1.00 20.33      B   C
ATOM  2760 CD1 ILE B  97     -9.130  86.028  42.048  1.00 18.39      B   C
ATOM  2761 C   ILE B  97     -9.985  90.408  41.741  1.00 20.42      B   C
ATOM  2762 O   ILE B  97    -10.881  90.502  40.904  1.00 21.88      B   O
ATOM  2763 N   LEU B  98     -9.670  91.393  42.575  1.00 22.89      B   N
ATOM  2764 CA  LEU B  98    -10.378  92.668  42.561  1.00 22.94      B   C
ATOM  2765 CB  LEU B  98     -9.918  93.539  43.734  1.00 24.42      B   C
ATOM  2766 CG  LEU B  98    -10.197  92.998  45.143  1.00 24.87      B   C
ATOM  2767 CD1 LEU B  98     -9.532  93.893  46.172  1.00 27.53      B   C
ATOM  2768 CD2 LEU B  98    -11.701  92.922  45.389  1.00 25.92      B   C
ATOM  2769 C   LEU B  98    -10.150  93.411  41.249  1.00 23.55      B   C
ATOM  2770 O   LEU B  98    -11.067  94.032  40.708  1.00 24.17      B   O
ATOM  2771 N   ALA B  99     -8.924  93.351  40.740  1.00 23.11      B   N
ATOM  2772 CA  ALA B  99     -8.594  94.025  39.491  1.00 22.89      B   C
ATOM  2773 CB  ALA B  99     -7.110  93.904  39.208  1.00 22.27      B   C
ATOM  2774 C   ALA B  99     -9.390  93.395  38.362  1.00 21.70      B   C
ATOM  2775 O   ALA B  99     -9.921  94.090  37.497  1.00 18.65      B   O
ATOM  2776 N   ILE B 100     -9.457  92.068  38.377  1.00 19.64      B   N
ATOM  2777 CA  ILE B 100    -10.190  91.331  37.363  1.00 19.82      B   C
ATOM  2778 CB  ILE B 100    -10.044  89.803  37.568  1.00 21.33      B   C
ATOM  2779 CG2 ILE B 100    -11.118  89.054  36.784  1.00 19.75      B   C
ATOM  2780 CG1 ILE B 100     -8.644  89.357  37.134  1.00 20.47      B   C
ATOM  2781 CD1 ILE B 100     -8.425  87.859  37.227  1.00 23.03      B   C
ATOM  2782 C   ILE B 100    -11.664  91.717  37.413  1.00 20.18      B   C
ATOM  2783 O   ILE B 100    -12.310  91.842  36.378  1.00 17.92      B   O
ATOM  2784 N   LYS B 101    -12.192  91.910  38.617  1.00 21.96      B   N
ATOM  2785 CA  LYS B 101    -13.594  92.296  38.755  1.00 24.71      B   C
ATOM  2786 CB  LYS B 101    -13.980  92.434  40.229  1.00 25.47      B   C
ATOM  2787 CG  LYS B 101    -14.034  91.120  40.988  1.00 30.47      B   C
ATOM  2788 CD  LYS B 101    -14.348  91.358  42.460  1.00 36.47      B   C
ATOM  2789 CE  LYS B 101    -15.720  91.992  42.654  1.00 39.30      B   C
ATOM  2790 NZ  LYS B 101    -15.973  92.336  44.087  1.00 42.89      B   N
ATOM  2791 C   LYS B 101    -13.831  93.623  38.041  1.00 24.26      B   C
ATOM  2792 O   LYS B 101    -14.846  93.797  37.369  1.00 25.28      B   O
ATOM  2793 N   ARG B 102    -12.886  94.548  38.185  1.00 23.53      B   N
ATOM  2794 CA  ARG B 102    -12.986  95.865  37.559  1.00 24.45      B   C
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Figure 5XX

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ATOM  2795  CB  ARG B 102     -11.976  96.835  38.182  1.00 24.23      B   C
ATOM  2796  CG  ARG B 102     -12.234  97.217  39.625  1.00 25.40      B   C
ATOM  2797  CD  ARG B 102     -11.276  98.316  40.054  1.00 26.37      B   C
ATOM  2798  NE  ARG B 102      -9.888  97.863  40.086  1.00 27.81      B   N
ATOM  2799  CZ  ARG B 102      -9.328  97.229  41.114  1.00 27.91      B   C
ATOM  2800  NH1 ARG B 102     -10.035  96.972  42.206  1.00 27.77      B   N
ATOM  2801  NH2 ARG B 102      -8.058  96.857  41.051  1.00 22.49      B   N
ATOM  2802  C   ARG B 102     -12.747  95.846  36.051  1.00 23.56      B   C
ATOM  2803  O   ARG B 102     -13.394  96.576  35.306  1.00 21.65      B   O
ATOM  2804  N   GLN B 103     -11.816  95.010  35.605  1.00 22.46      B   N
ATOM  2805  CA  GLN B 103     -11.474  94.951  34.189  1.00 22.58      B   C
ATOM  2806  CB  GLN B 103      -9.972  94.728  34.036  1.00 21.32      B   C
ATOM  2807  CG  GLN B 103      -9.126  95.766  34.733  1.00 22.61      B   C
ATOM  2808  CD  GLN B 103      -7.659  95.405  34.712  1.00 22.94      B   C
ATOM  2809  OE1 GLN B 103      -7.074  95.216  33.647  1.00 24.42      B   O
ATOM  2810  NE2 GLN B 103      -7.055  95.305  35.890  1.00 22.74      B   N
ATOM  2811  C   GLN B 103     -12.206  93.918  33.349  1.00 22.98      B   C
ATOM  2812  O   GLN B 103     -12.221  94.020  32.126  1.00 23.73      B   O
ATOM  2813  N   VAL B 104     -12.807  92.925  33.989  1.00 22.89      B   N
ATOM  2814  CA  VAL B 104     -13.500  91.881  33.241  1.00 24.65      B   C
ATOM  2815  CB  VAL B 104     -12.796  90.518  33.427  1.00 25.96      B   C
ATOM  2816  CG1 VAL B 104     -13.465  89.462  32.568  1.00 25.99      B   C
ATOM  2817  CG2 VAL B 104     -11.321  90.643  33.066  1.00 24.05      B   C
ATOM  2818  C   VAL B 104     -14.957  91.752  33.663  1.00 26.14      B   C
ATOM  2819  O   VAL B 104     -15.284  90.975  34.557  1.00 23.04      B   O
ATOM  2820  N   GLU B 105     -15.821  92.515  33.000  1.00 28.13      B   N
ATOM  2821  CA  GLU B 105     -17.253  92.520  33.289  1.00 31.78      B   C
ATOM  2822  CB  GLU B 105     -17.923  93.703  32.581  1.00 37.19      B   C
ATOM  2823  CG  GLU B 105     -17.318  95.053  32.940  1.00 47.02      B   C
ATOM  2824  CD  GLU B 105     -17.983  96.226  32.231  1.00 50.74      B   C
ATOM  2825  OE1 GLU B 105     -18.016  96.247  30.979  1.00 51.99      B   O
ATOM  2826  OE2 GLU B 105     -18.469  97.136  32.933  1.00 54.70      B   O
ATOM  2827  C   GLU B 105     -17.953  91.231  32.877  1.00 29.48      B   C
ATOM  2828  O   GLU B 105     -18.915  90.807  33.518  1.00 32.30      B   O
ATOM  2829  N   ASP B 106     -17.471  90.608  31.808  1.00 27.12      B   N
ATOM  2830  CA  ASP B 106     -18.067  89.377  31.310  1.00 26.01      B   C
ATOM  2831  CB  ASP B 106     -17.666  89.167  29.850  1.00 26.98      B   C
ATOM  2832  CG  ASP B 106     -18.215  87.881  29.272  1.00 28.23      B   C
ATOM  2833  OD1 ASP B 106     -19.054  87.232  29.930  1.00 28.83      B   O
ATOM  2834  OD2 ASP B 106     -17.807  87.521  28.147  1.00 31.85      B   O
ATOM  2835  C   ASP B 106     -17.666  88.168  32.147  1.00 25.85      B   C
ATOM  2836  O   ASP B 106     -16.517  87.736  32.118  1.00 24.84      B   O
ATOM  2837  N   LYS B 107     -18.628  87.626  32.890  1.00 25.49      B   N
ATOM  2838  CA  LYS B 107     -18.396  86.472  33.754  1.00 27.31      B   C
ATOM  2839  CB  LYS B 107     -19.633  86.210  34.622  1.00 29.26      B   C
ATOM  2840  CG  LYS B 107     -19.948  87.328  35.600  1.00 32.01      B   C
ATOM  2841  CD  LYS B 107     -18.757  87.611  36.512  1.00 33.91      B   C
ATOM  2842  CE  LYS B 107     -19.056  88.718  37.516  1.00 34.29      B   C
ATOM  2843  NZ  LYS B 107     -19.369  90.016  36.853  1.00 41.19      B   N
ATOM  2844  C   LYS B 107     -18.044  85.203  32.991  1.00 26.67      B   C
ATOM  2845  O   LYS B 107     -17.508  84.254  33.565  1.00 28.78      B   O
ATOM  2846  N   ASN B 108     -18.337  85.187  31.698  1.00 26.36      B   N
ATOM  2847  CA  ASN B 108     -18.059  84.019  30.875  1.00 27.30      B   C
ATOM  2848  CB  ASN B 108     -19.176  83.833  29.848  1.00 32.21      B   C
ATOM  2849  CG  ASN B 108     -20.509  83.515  30.496  1.00 37.21      B   C
ATOM  2850  OD1 ASN B 108     -20.670  82.470  31.130  1.00 41.66      B   O
ATOM  2851  ND2 ASN B 108     -21.473  84.420  30.350  1.00 39.88      B   N
ATOM  2852  C   ASN B 108     -16.719  84.106  30.160  1.00 25.00      B   C
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Figure 5YY

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ATOM  2853  O   ASN B 108    -16.318  83.173  29.467  1.00 27.12    B   O
ATOM  2854  N   ALA B 109    -16.029  85.227  30.333  1.00 22.44    B   N
ATOM  2855  CA  ALA B 109    -14.734  85.427  29.696  1.00 22.32    B   C
ATOM  2856  CB  ALA B 109    -14.179  86.795  30.062  1.00 19.60    B   C
ATOM  2857  C   ALA B 109    -13.768  84.334  30.133  1.00 21.09    B   C
ATOM  2858  O   ALA B 109    -13.580  84.107  31.326  1.00 21.33    B   O
ATOM  2859  N   PRO B 110    -13.152  83.635  29.168  1.00 21.10    B   N
ATOM  2860  CD  PRO B 110    -13.315  83.775  27.711  1.00 21.88    B   C
ATOM  2861  CA  PRO B 110    -12.201  82.562  29.485  1.00 21.55    B   C
ATOM  2862  CB  PRO B 110    -11.843  81.988  28.111  1.00 20.46    B   C
ATOM  2863  CG  PRO B 110    -13.002  82.387  27.233  1.00 23.31    B   C
ATOM  2864  C   PRO B 110    -10.974  83.142  30.190  1.00 21.39    B   C
ATOM  2865  O   PRO B 110    -10.243  83.950  29.615  1.00 20.23    B   O
ATOM  2866  N   ILE B 111    -10.757  82.731  31.433  1.00 20.74    B   N
ATOM  2867  CA  ILE B 111     -9.621  83.220  32.208  1.00 21.29    B   C
ATOM  2868  CB  ILE B 111    -10.085  83.770  33.575  1.00 18.70    B   C
ATOM  2869  CG2 ILE B 111     -8.883  84.214  34.398  1.00 19.35    B   C
ATOM  2870  CG1 ILE B 111    -11.054  84.937  33.365  1.00 17.87    B   C
ATOM  2871  CD1 ILE B 111    -11.768  85.374  34.632  1.00 13.74    B   C
ATOM  2872  C   ILE B 111     -8.618  82.096  32.439  1.00 20.50    B   C
ATOM  2873  O   ILE B 111     -8.983  81.017  32.900  1.00 21.37    B   O
ATOM  2874  N   LEU B 112     -7.358  82.354  32.107  1.00 19.57    B   N
ATOM  2875  CA  LEU B 112     -6.302  81.367  32.285  1.00 18.55    B   C
ATOM  2876  CB  LEU B 112     -5.538  81.154  30.975  1.00 17.95    B   C
ATOM  2877  CG  LEU B 112     -4.340  80.200  31.024  1.00 18.08    B   C
ATOM  2878  CD1 LEU B 112     -4.774  78.812  31.482  1.00 19.26    B   C
ATOM  2879  CD2 LEU B 112     -3.713  80.132  29.640  1.00 16.52    B   C
ATOM  2880  C   LEU B 112     -5.329  81.799  33.370  1.00 18.08    B   C
ATOM  2881  O   LEU B 112     -4.731  82.873  33.291  1.00 19.20    B   O
ATOM  2882  N   VAL B 113     -5.171  80.951  34.380  1.00 16.92    B   N
ATOM  2883  CA  VAL B 113     -4.269  81.231  35.487  1.00 16.68    B   C
ATOM  2884  CB  VAL B 113     -4.863  80.728  36.835  1.00 17.69    B   C
ATOM  2885  CG1 VAL B 113     -3.945  81.110  37.994  1.00 17.55    B   C
ATOM  2886  CG2 VAL B 113     -6.244  81.309  37.050  1.00 17.01    B   C
ATOM  2887  C   VAL B 113     -2.943  80.516  35.243  1.00 16.02    B   C
ATOM  2888  O   VAL B 113     -2.921  79.308  34.999  1.00 14.64    B   O
ATOM  2889  N   LEU B 114     -1.845  81.267  35.291  1.00 14.63    B   N
ATOM  2890  CA  LEU B 114     -0.520  80.692  35.104  1.00 13.92    B   C
ATOM  2891  CB  LEU B 114      0.247  81.395  33.979  1.00 11.65    B   C
ATOM  2892  CG  LEU B 114     -0.330  81.466  32.566  1.00 17.67    B   C
ATOM  2893  CD1 LEU B 114      0.736  82.064  31.644  1.00 16.72    B   C
ATOM  2894  CD2 LEU B 114     -0.738  80.081  32.077  1.00 17.71    B   C
ATOM  2895  C   LEU B 114      0.256  80.881  36.399  1.00 14.25    B   C
ATOM  2896  O   LEU B 114      0.210  81.947  37.005  1.00 11.47    B   O
ATOM  2897  N   GLY B 115      0.984  79.855  36.813  1.00 14.70    B   N
ATOM  2898  CA  GLY B 115      1.757  79.971  38.037  1.00 15.73    B   C
ATOM  2899  C   GLY B 115      2.608  78.746  38.289  1.00 14.74    B   C
ATOM  2900  O   GLY B 115      2.693  77.855  37.451  1.00 13.78    B   O
ATOM  2901  N   THR B 116      3.252  78.706  39.447  1.00 16.02    B   N
ATOM  2902  CA  THR B 116      4.087  77.568  39.798  1.00 15.11    B   C
ATOM  2903  CB  THR B 116      4.916  77.860  41.045  1.00 14.07    B   C
ATOM  2904  OG1 THR B 116      4.040  78.104  42.155  1.00 12.96    B   O
ATOM  2905  CG2 THR B 116      5.800  79.074  40.814  1.00 13.81    B   C
ATOM  2906  C   THR B 116      3.182  76.375  40.083  1.00 15.15    B   C
ATOM  2907  O   THR B 116      1.974  76.528  40.260  1.00 15.43    B   O
ATOM  2908  N   LYS B 117      3.768  75.189  40.124  1.00 14.92    B   N
ATOM  2909  CA  LYS B 117      2.998  73.991  40.401  1.00 16.68    B   C
ATOM  2910  CB  LYS B 117      3.926  72.776  40.462  1.00 18.20    B   C
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Figure 5ZZ

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ATOM  2911 CG  LYS B 117     3.170  71.459  40.516  1.00 28.15    B   C
ATOM  2912 CD  LYS B 117     2.286  71.334  39.280  1.00 34.68    B   C
ATOM  2913 CE  LYS B 117     1.422  70.089  39.310  1.00 37.95    B   C
ATOM  2914 NZ  LYS B 117     0.628  69.995  38.057  1.00 40.68    B   N
ATOM  2915 C   LYS B 117     2.231  74.125  41.725  1.00 15.54    B   C
ATOM  2916 O   LYS B 117     1.055  73.772  41.811  1.00 13.25    B   O
ATOM  2917 N   ALA B 118     2.896  74.648  42.753  1.00 13.55    B   N
ATOM  2918 CA  ALA B 118     2.263  74.797  44.062  1.00 13.07    B   C
ATOM  2919 CB  ALA B 118     3.294  75.271  45.092  1.00 13.77    B   C
ATOM  2920 C   ALA B 118     1.084  75.755  44.020  1.00 13.96    B   C
ATOM  2921 O   ALA B 118     0.022  75.478  44.584  1.00 12.32    B   O
ATOM  2922 N   THR B 119     1.270  76.887  43.347  1.00 12.40    B   N
ATOM  2923 CA  THR B 119     0.204  77.874  43.248  1.00 14.50    B   C
ATOM  2924 CB  THR B 119     0.698  79.159  42.534  1.00 11.89    B   C
ATOM  2925 OG1 THR B 119     1.739  79.763  43.311  1.00 13.56    B   O
ATOM  2926 CG2 THR B 119    -0.443  80.158  42.373  1.00 12.19    B   C
ATOM  2927 C   THR B 119    -1.005  77.312  42.504  1.00 12.61    B   C
ATOM  2928 O   THR B 119    -2.140  77.473  42.942  1.00 15.20    B   O
ATOM  2929 N   ILE B 120    -0.759  76.641  41.385  1.00 13.07    B   N
ATOM  2930 CA  ILE B 120    -1.847  76.080  40.594  1.00 17.11    B   C
ATOM  2931 CB  ILE B 120    -1.333  75.521  39.242  1.00 15.75    B   C
ATOM  2932 CG2 ILE B 120    -2.499  74.993  38.418  1.00 19.67    B   C
ATOM  2933 CG1 ILE B 120    -0.600  76.620  38.461  1.00 15.38    B   C
ATOM  2934 CD1 ILE B 120    -1.456  77.829  38.120  1.00 19.05    B   C
ATOM  2935 C   ILE B 120    -2.605  74.971  41.331  1.00 17.21    B   C
ATOM  2936 O   ILE B 120    -3.832  74.938  41.309  1.00 18.55    B   O
ATOM  2937 N   GLN B 121    -1.887  74.064  41.984  1.00 17.85    B   N
ATOM  2938 CA  GLN B 121    -2.554  72.983  42.700  1.00 21.02    B   C
ATOM  2939 CB  GLN B 121    -1.539  71.946  43.177  1.00 23.26    B   C
ATOM  2940 CG  GLN B 121    -0.796  71.267  42.053  1.00 31.27    B   C
ATOM  2941 CD  GLN B 121    -0.046  70.038  42.509  1.00 34.42    B   C
ATOM  2942 OE1 GLN B 121     0.702  70.078  43.488  1.00 38.77    B   O
ATOM  2943 NE2 GLN B 121    -0.237  68.933  41.797  1.00 36.80    B   N
ATOM  2944 C   GLN B 121    -3.375  73.477  43.894  1.00 21.84    B   C
ATOM  2945 O   GLN B 121    -4.297  72.795  44.345  1.00 23.51    B   O
ATOM  2946 N   SER B 122    -3.056  74.661  44.404  1.00 20.44    B   N
ATOM  2947 CA  SER B 122    -3.791  75.193  45.549  1.00 20.89    B   C
ATOM  2948 CB  SER B 122    -3.024  76.348  46.208  1.00 20.03    B   C
ATOM  2949 OG  SER B 122    -3.115  77.537  45.438  1.00 19.77    B   O
ATOM  2950 C   SER B 122    -5.178  75.687  45.152  1.00 19.13    B   C
ATOM  2951 O   SER B 122    -6.057  75.812  46.000  1.00 18.67    B   O
ATOM  2952 N   ASN B 123    -5.362  75.960  43.864  1.00 20.34    B   N
ATOM  2953 CA  ASN B 123    -6.626  76.476  43.345  1.00 21.65    B   C
ATOM  2954 CB  ASN B 123    -7.756  75.464  43.543  1.00 24.19    B   C
ATOM  2955 CG  ASN B 123    -7.662  74.302  42.583  1.00 28.22    B   C
ATOM  2956 OD1 ASN B 123    -7.618  74.492  41.368  1.00 28.03    B   O
ATOM  2957 ND2 ASN B 123    -7.632  73.087  43.121  1.00 31.95    B   N
ATOM  2958 C   ASN B 123    -6.990  77.787  44.025  1.00 20.93    B   C
ATOM  2959 O   ASN B 123    -8.162  78.160  44.098  1.00 20.81    B   O
ATOM  2960 N   ALA B 124    -5.977  78.488  44.520  1.00 18.37    B   N
ATOM  2961 CA  ALA B 124    -6.205  79.759  45.187  1.00 19.77    B   C
ATOM  2962 CB  ALA B 124    -4.872  80.387  45.588  1.00 18.94    B   C
ATOM  2963 C   ALA B 124    -6.993  80.715  44.285  1.00 18.40    B   C
ATOM  2964 O   ALA B 124    -8.032  81.239  44.685  1.00 20.72    B   O
ATOM  2965 N   TYR B 125    -6.506  80.936  43.069  1.00 19.24    B   N
ATOM  2966 CA  TYR B 125    -7.184  81.841  42.142  1.00 19.32    B   C
ATOM  2967 CB  TYR B 125    -6.331  82.091  40.892  1.00 19.37    B   C
ATOM  2968 CG  TYR B 125    -5.129  82.989  41.102  1.00 19.31    B   C
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Figure 5AAA

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ATOM  2969 CD1 TYR B 125     -3.887  82.457  41.439  1.00 17.61      B   C
ATOM  2970 CE1 TYR B 125     -2.768  83.280  41.591  1.00 18.62      B   C
ATOM  2971 CD2 TYR B 125     -5.228  84.371  40.929  1.00 17.15      B   C
ATOM  2972 CE2 TYR B 125     -4.123  85.197  41.078  1.00 16.64      B   C
ATOM  2973 CZ  TYR B 125     -2.895  84.646  41.405  1.00 17.43      B   C
ATOM  2974 OH  TYR B 125     -1.792  85.454  41.520  1.00 17.10      B   O
ATOM  2975 C   TYR B 125     -8.553  81.340  41.696  1.00 19.25      B   C
ATOM  2976 O   TYR B 125     -9.528  82.096  41.688  1.00 18.74      B   O
ATOM  2977 N   ASP B 126     -8.617  80.071  41.310  1.00 18.47      B   N
ATOM  2978 CA  ASP B 126     -9.862  79.473  40.841  1.00 19.68      B   C
ATOM  2979 CB  ASP B 126     -9.660  77.986  40.552  1.00 19.72      B   C
ATOM  2980 CG  ASP B 126     -8.455  77.720  39.671  1.00 23.51      B   C
ATOM  2981 OD1 ASP B 126     -7.341  78.138  40.042  1.00 24.96      B   O
ATOM  2982 OD2 ASP B 126     -8.621  77.085  38.609  1.00 22.93      B   O
ATOM  2983 C   ASP B 126    -10.972  79.635  41.868  1.00 21.84      B   C
ATOM  2984 O   ASP B 126    -12.076  80.077  41.541  1.00 18.17      B   O
ATOM  2985 N   ASN B 127    -10.676  79.273  43.113  1.00 21.58      B   N
ATOM  2986 CA  ASN B 127    -11.659  79.376  44.181  1.00 22.68      B   C
ATOM  2987 CB  ASN B 127    -11.081  78.839  45.495  1.00 22.98      B   C
ATOM  2988 CG  ASN B 127    -10.656  77.385  45.393  1.00 26.68      B   C
ATOM  2989 OD1 ASN B 127    -11.290  76.591  44.701  1.00 26.92      B   O
ATOM  2990 ND2 ASN B 127     -9.582  77.029  46.092  1.00 29.75      B   N
ATOM  2991 C   ASN B 127    -12.105  80.821  44.362  1.00 22.20      B   C
ATOM  2992 O   ASN B 127    -13.300  81.104  44.443  1.00 22.96      B   O
ATOM  2993 N   ALA B 128    -11.145  81.736  44.422  1.00 21.77      B   N
ATOM  2994 CA  ALA B 128    -11.465  83.149  44.587  1.00 22.81      B   C
ATOM  2995 CB  ALA B 128    -10.184  83.970  44.693  1.00 24.04      B   C
ATOM  2996 C   ALA B 128    -12.315  83.643  43.422  1.00 24.10      B   C
ATOM  2997 O   ALA B 128    -13.302  84.354  43.624  1.00 27.04      B   O
ATOM  2998 N   LEU B 129    -11.935  83.262  42.205  1.00 24.54      B   N
ATOM  2999 CA  LEU B 129    -12.672  83.664  41.012  1.00 24.58      B   C
ATOM  3000 CB  LEU B 129    -11.926  83.225  39.753  1.00 22.03      B   C
ATOM  3001 CG  LEU B 129    -10.633  83.975  39.418  1.00 24.03      B   C
ATOM  3002 CD1 LEU B 129     -9.865  83.210  38.366  1.00 22.36      B   C
ATOM  3003 CD2 LEU B 129    -10.956  85.382  38.932  1.00 22.58      B   C
ATOM  3004 C   LEU B 129    -14.078  83.070  41.005  1.00 26.08      B   C
ATOM  3005 O   LEU B 129    -15.046  83.751  40.669  1.00 26.16      B   O
ATOM  3006 N   LYS B 130    -14.185  81.795  41.365  1.00 26.80      B   N
ATOM  3007 CA  LYS B 130    -15.482  81.130  41.404  1.00 29.37      B   C
ATOM  3008 CB  LYS B 130    -15.326  79.694  41.904  1.00 32.59      B   C
ATOM  3009 CG  LYS B 130    -16.638  78.939  42.019  1.00 37.42      B   C
ATOM  3010 CD  LYS B 130    -17.337  78.877  40.675  1.00 43.42      B   C
ATOM  3011 CE  LYS B 130    -18.708  78.237  40.775  1.00 45.02      B   C
ATOM  3012 NZ  LYS B 130    -19.379  78.220  39.444  1.00 49.29      B   N
ATOM  3013 C   LYS B 130    -16.400  81.897  42.347  1.00 29.56      B   C
ATOM  3014 O   LYS B 130    -17.538  82.218  42.010  1.00 28.29      B   O
ATOM  3015 N   GLN B 131    -15.876  82.185  43.532  1.00 29.31      B   N
ATOM  3016 CA  GLN B 131    -16.599  82.911  44.559  1.00 31.88      B   C
ATOM  3017 CB  GLN B 131    -15.667  83.162  45.747  1.00 35.97      B   C
ATOM  3018 CG  GLN B 131    -16.286  83.913  46.918  1.00 45.23      B   C
ATOM  3019 CD  GLN B 131    -17.385  83.128  47.610  1.00 50.61      B   C
ATOM  3020 OE1 GLN B 131    -17.211  81.951  47.942  1.00 53.57      B   O
ATOM  3021 NE2 GLN B 131    -18.524  83.781  47.843  1.00 52.00      B   N
ATOM  3022 C   GLN B 131    -17.137  84.239  44.035  1.00 31.40      B   C
ATOM  3023 O   GLN B 131    -18.222  84.675  44.427  1.00 29.81      B   O
ATOM  3024 N   GLN B 132    -16.382  84.878  43.145  1.00 29.49      B   N
ATOM  3025 CA  GLN B 132    -16.788  86.166  42.597  1.00 29.13      B   C
ATOM  3026 CB  GLN B 132    -15.558  87.020  42.290  1.00 30.78      B   C
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Figure 5BBB

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ATOM  3027  CG  GLN B 132    -14.776  87.410  43.535  1.00 32.44    B   C
ATOM  3028  CD  GLN B 132    -15.644  88.114  44.565  1.00 35.76    B   C
ATOM  3029  OE1 GLN B 132    -16.234  89.158  44.286  1.00 35.79    B   O
ATOM  3030  NE2 GLN B 132    -15.725  87.542  45.763  1.00 34.46    B   N
ATOM  3031  C   GLN B 132    -17.682  86.079  41.368  1.00 29.17    B   C
ATOM  3032  O   GLN B 132    -17.994  87.096  40.747  1.00 28.85    B   O
ATOM  3033  N   GLY B 133    -18.075  84.864  41.004  1.00 28.71    B   N
ATOM  3034  CA  GLY B 133    -18.974  84.700  39.879  1.00 28.15    B   C
ATOM  3035  C   GLY B 133    -18.442  84.343  38.509  1.00 27.61    B   C
ATOM  3036  O   GLY B 133    -19.224  84.310  37.561  1.00 26.00    B   O
ATOM  3037  N   TYR B 134    -17.146  84.078  38.371  1.00 26.83    B   N
ATOM  3038  CA  TYR B 134    -16.627  83.721  37.056  1.00 26.16    B   C
ATOM  3039  CB  TYR B 134    -15.135  84.049  36.961  1.00 24.55    B   C
ATOM  3040  CG  TYR B 134    -14.921  85.545  36.938  1.00 22.77    B   C
ATOM  3041  CD1 TYR B 134    -14.840  86.277  38.123  1.00 22.62    B   C
ATOM  3042  CE1 TYR B 134    -14.760  87.670  38.109  1.00 23.49    B   C
ATOM  3043  CD2 TYR B 134    -14.911  86.246  35.730  1.00 24.51    B   C
ATOM  3044  CE2 TYR B 134    -14.834  87.641  35.702  1.00 25.08    B   C
ATOM  3045  CZ  TYR B 134    -14.759  88.346  36.896  1.00 23.66    B   C
ATOM  3046  OH  TYR B 134    -14.689  89.721  36.886  1.00 24.39    B   O
ATOM  3047  C   TYR B 134    -16.927  82.264  36.729  1.00 26.95    B   C
ATOM  3048  O   TYR B 134    -16.774  81.379  37.571  1.00 26.50    B   O
ATOM  3049  N   LEU B 135    -17.362  82.031  35.494  1.00 25.91    B   N
ATOM  3050  CA  LEU B 135    -17.777  80.704  35.049  1.00 28.31    B   C
ATOM  3051  CB  LEU B 135    -19.155  80.822  34.388  1.00 28.49    B   C
ATOM  3052  CG  LEU B 135    -20.131  81.733  35.139  1.00 28.21    B   C
ATOM  3053  CD1 LEU B 135    -21.343  82.031  34.272  1.00 28.13    B   C
ATOM  3054  CD2 LEU B 135    -20.527  81.077  36.455  1.00 29.07    B   C
ATOM  3055  C   LEU B 135    -16.847  79.940  34.113  1.00 27.36    B   C
ATOM  3056  O   LEU B 135    -17.066  78.758  33.855  1.00 27.87    B   O
ATOM  3057  N   ASN B 136    -15.819  80.602  33.596  1.00 28.12    B   N
ATOM  3058  CA  ASN B 136    -14.892  79.944  32.681  1.00 25.99    B   C
ATOM  3059  CB  ASN B 136    -15.053  80.520  31.276  1.00 27.18    B   C
ATOM  3060  CG  ASN B 136    -14.416  79.652  30.214  1.00 27.92    B   C
ATOM  3061  OD1 ASN B 136    -13.572  78.807  30.509  1.00 28.48    B   O
ATOM  3062  ND2 ASN B 136    -14.809  79.866  28.962  1.00 30.11    B   N
ATOM  3063  C   ASN B 136    -13.460  80.159  33.172  1.00 26.03    B   C
ATOM  3064  O   ASN B 136    -12.749  81.040  32.688  1.00 24.61    B   O
ATOM  3065  N   ILE B 137    -13.046  79.342  34.133  1.00 24.40    B   N
ATOM  3066  CA  ILE B 137    -11.715  79.451  34.716  1.00 24.19    B   C
ATOM  3067  CB  ILE B 137    -11.816  79.575  36.254  1.00 25.00    B   C
ATOM  3068  CG2 ILE B 137    -10.430  79.802  36.857  1.00 26.36    B   C
ATOM  3069  CG1 ILE B 137    -12.752  80.735  36.616  1.00 25.12    B   C
ATOM  3070  CD1 ILE B 137    -13.231  80.738  38.056  1.00 25.56    B   C
ATOM  3071  C   ILE B 137    -10.809  78.268  34.378  1.00 24.30    B   C
ATOM  3072  O   ILE B 137    -11.180  77.114  34.574  1.00 24.24    B   O
ATOM  3073  N   SER B 138     -9.620  78.570  33.865  1.00 22.99    B   N
ATOM  3074  CA  SER B 138     -8.640  77.545  33.520  1.00 23.07    B   C
ATOM  3075  CB  SER B 138     -8.357  77.547  32.016  1.00 21.90    B   C
ATOM  3076  OG  SER B 138     -9.532  77.297  31.271  1.00 28.80    B   O
ATOM  3077  C   SER B 138     -7.345  77.845  34.267  1.00 21.12    B   C
ATOM  3078  O   SER B 138     -7.104  78.986  34.675  1.00 18.88    B   O
ATOM  3079  N   HIS B 139     -6.521  76.820  34.463  1.00 20.44    B   N
ATOM  3080  CA  HIS B 139     -5.242  77.010  35.134  1.00 20.66    B   C
ATOM  3081  CB  HIS B 139     -5.343  76.712  36.639  1.00 20.23    B   C
ATOM  3082  CG  HIS B 139     -5.802  75.322  36.964  1.00 21.50    B   C
ATOM  3083  CD2 HIS B 139     -5.241  74.114  36.716  1.00 22.63    B   C
ATOM  3084  ND1 HIS B 139     -6.984  75.067  37.626  1.00 20.86    B   N
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Figure 5CCC

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ATOM  3085 CE1 HIS B 139    -7.132  73.761  37.770  1.00 23.65    B   C
ATOM  3086 NE2 HIS B 139    -6.089  73.161  37.226  1.00 23.23    B   N
ATOM  3087 C   HIS B 139    -4.172  76.148  34.488  1.00 21.34    B   C
ATOM  3088 O   HIS B 139    -4.468  75.120  33.874  1.00 21.81    B   O
ATOM  3089 N   LEU B 140    -2.922  76.578  34.614  1.00 21.36    B   N
ATOM  3090 CA  LEU B 140    -1.815  75.846  34.023  1.00 20.20    B   C
ATOM  3091 CB  LEU B 140    -1.644  76.244  32.558  1.00 21.19    B   C
ATOM  3092 CG  LEU B 140    -0.502  75.564  31.800  1.00 21.50    B   C
ATOM  3093 CD1 LEU B 140    -0.790  74.074  31.688  1.00 21.95    B   C
ATOM  3094 CD2 LEU B 140    -0.357  76.190  30.410  1.00 21.96    B   C
ATOM  3095 C   LEU B 140    -0.511  76.104  34.758  1.00 19.11    B   C
ATOM  3096 O   LEU B 140    -0.098  77.248  34.928  1.00 16.59    B   O
ATOM  3097 N   ALA B 141     0.135  75.027  35.186  1.00 19.36    B   N
ATOM  3098 CA  ALA B 141     1.405  75.133  35.887  1.00 19.87    B   C
ATOM  3099 CB  ALA B 141     1.603  73.918  36.791  1.00 21.48    B   C
ATOM  3100 C   ALA B 141     2.531  75.215  34.856  1.00 16.62    B   C
ATOM  3101 O   ALA B 141     2.912  74.214  34.261  1.00 20.61    B   O
ATOM  3102 N   THR B 142     3.049  76.415  34.630  1.00 15.84    B   N
ATOM  3103 CA  THR B 142     4.132  76.600  33.676  1.00 14.20    B   C
ATOM  3104 CB  THR B 142     3.948  77.913  32.889  1.00 13.97    B   C
ATOM  3105 OG1 THR B 142     3.814  79.003  33.806  1.00 14.25    B   O
ATOM  3106 CG2 THR B 142     2.691  77.840  32.023  1.00 13.62    B   C
ATOM  3107 C   THR B 142     5.410  76.652  34.505  1.00 14.37    B   C
ATOM  3108 O   THR B 142     6.114  77.653  34.529  1.00 13.97    B   O
ATOM  3109 N   SER B 143     5.698  75.544  35.176  1.00 15.59    B   N
ATOM  3110 CA  SER B 143     6.844  75.444  36.067  1.00 16.89    B   C
ATOM  3111 CB  SER B 143     6.971  74.013  36.591  1.00 19.31    B   C
ATOM  3112 OG  SER B 143     8.003  73.931  37.564  1.00 27.09    B   O
ATOM  3113 C   SER B 143     8.193  75.902  35.537  1.00 16.21    B   C
ATOM  3114 O   SER B 143     8.892  76.666  36.205  1.00 16.07    B   O
ATOM  3115 N   LEU B 144     8.557  75.446  34.345  1.00 15.08    B   N
ATOM  3116 CA  LEU B 144     9.850  75.783  33.759  1.00 15.48    B   C
ATOM  3117 CB  LEU B 144    10.094  74.929  32.520  1.00 15.32    B   C
ATOM  3118 CG  LEU B 144    10.215  73.436  32.827  1.00 16.70    B   C
ATOM  3119 CD1 LEU B 144    10.267  72.642  31.536  1.00 19.80    B   C
ATOM  3120 CD2 LEU B 144    11.468  73.190  33.654  1.00 19.07    B   C
ATOM  3121 C   LEU B 144    10.037  77.251  33.421  1.00 14.68    B   C
ATOM  3122 O   LEU B 144    11.145  77.678  33.098  1.00 14.35    B   O
ATOM  3123 N   PHE B 145     8.962  78.028  33.484  1.00 14.12    B   N
ATOM  3124 CA  PHE B 145     9.088  79.447  33.199  1.00 15.35    B   C
ATOM  3125 CB  PHE B 145     7.719  80.148  33.232  1.00 13.56    B   C
ATOM  3126 CG  PHE B 145     6.911  79.992  31.964  1.00 14.58    B   C
ATOM  3127 CD1 PHE B 145     5.657  80.594  31.852  1.00 13.83    B   C
ATOM  3128 CD2 PHE B 145     7.393  79.252  30.888  1.00 16.08    B   C
ATOM  3129 CE1 PHE B 145     4.899  80.461  30.688  1.00 14.15    B   C
ATOM  3130 CE2 PHE B 145     6.646  79.111  29.720  1.00 15.95    B   C
ATOM  3131 CZ  PHE B 145     5.395  79.717  29.620  1.00 14.39    B   C
ATOM  3132 C   PHE B 145    10.011  80.084  34.233  1.00 14.15    B   C
ATOM  3133 O   PHE B 145    10.821  80.942  33.896  1.00 13.84    B   O
ATOM  3134 N   VAL B 146     9.901  79.648  35.488  1.00 14.43    B   N
ATOM  3135 CA  VAL B 146    10.721  80.215  36.558  1.00 15.36    B   C
ATOM  3136 CB  VAL B 146    10.353  79.617  37.949  1.00 17.29    B   C
ATOM  3137 CG1 VAL B 146    11.367  80.065  38.995  1.00 16.50    B   C
ATOM  3138 CG2 VAL B 146     8.959  80.079  38.369  1.00 14.60    B   C
ATOM  3139 C   VAL B 146    12.229  80.086  36.329  1.00 14.39    B   C
ATOM  3140 O   VAL B 146    12.935  81.092  36.326  1.00 14.20    B   O
ATOM  3141 N   PRO B 147    12.747  78.856  36.144  1.00 14.14    B   N
ATOM  3142 CD  PRO B 147    12.141  77.519  36.269  1.00 13.43    B   C
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Figure 5DDD

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ATOM  3143 CA  PRO B 147     14.195  78.754  35.921  1.00 14.59      B   C
ATOM  3144 CB  PRO B 147     14.457  77.242  35.995  1.00 13.53      B   C
ATOM  3145 CG  PRO B 147     13.151  76.642  35.573  1.00 14.07      B   C
ATOM  3146 C   PRO B 147     14.653  79.377  34.597  1.00 13.40      B   C
ATOM  3147 O   PRO B 147     15.775  79.877  34.500  1.00 13.19      B   O
ATOM  3148 N   LEU B 148     13.796  79.355  33.577  1.00 11.38      B   N
ATOM  3149 CA  LEU B 148     14.179  79.960  32.303  1.00 12.63      B   C
ATOM  3150 CB  LEU B 148     13.100  79.751  31.232  1.00 14.70      B   C
ATOM  3151 CG  LEU B 148     13.404  78.655  30.202  1.00 12.09      B   C
ATOM  3152 CD1 LEU B 148     13.446  77.315  30.903  1.00 14.46      B   C
ATOM  3153 CD2 LEU B 148     12.341  78.649  29.106  1.00 18.20      B   C
ATOM  3154 C   LEU B 148     14.395  81.448  32.508  1.00 12.91      B   C
ATOM  3155 O   LEU B 148     15.372  82.018  32.031  1.00 12.96      B   O
ATOM  3156 N   ILE B 149     13.471  82.070  33.231  1.00 13.00      B   N
ATOM  3157 CA  ILE B 149     13.545  83.500  33.499  1.00 12.87      B   C
ATOM  3158 CB  ILE B 149     12.211  83.989  34.130  1.00 13.86      B   C
ATOM  3159 CG2 ILE B 149     12.352  85.419  34.647  1.00 12.28      B   C
ATOM  3160 CG1 ILE B 149     11.099  83.891  33.071  1.00 14.05      B   C
ATOM  3161 CD1 ILE B 149      9.694  84.067  33.608  1.00 15.21      B   C
ATOM  3162 C   ILE B 149     14.742  83.842  34.386  1.00 12.66      B   C
ATOM  3163 O   ILE B 149     15.403  84.852  34.172  1.00 11.51      B   O
ATOM  3164 N   GLU B 150     15.041  82.995  35.366  1.00 12.92      B   N
ATOM  3165 CA  GLU B 150     16.180  83.266  36.235  1.00 13.66      B   C
ATOM  3166 CB  GLU B 150     16.182  82.313  37.441  1.00 18.92      B   C
ATOM  3167 CG  GLU B 150     14.884  82.371  38.242  1.00 23.46      B   C
ATOM  3168 CD  GLU B 150     15.024  81.875  39.673  1.00 28.25      B   C
ATOM  3169 OE1 GLU B 150     15.728  80.863  39.887  1.00 30.76      B   O
ATOM  3170 OE2 GLU B 150     14.414  82.491  40.581  1.00 24.21      B   O
ATOM  3171 C   GLU B 150     17.491  83.163  35.462  1.00 13.99      B   C
ATOM  3172 O   GLU B 150     18.484  83.776  35.844  1.00 14.58      B   O
ATOM  3173 N   GLU B 151     17.500  82.403  34.370  1.00 13.36      B   N
ATOM  3174 CA  GLU B 151     18.712  82.277  33.571  1.00 16.12      B   C
ATOM  3175 CB  GLU B 151     18.863  80.861  33.006  1.00 18.99      B   C
ATOM  3176 CG  GLU B 151     20.276  80.598  32.500  1.00 25.66      B   C
ATOM  3177 CD  GLU B 151     20.615  79.128  32.403  1.00 27.80      B   C
ATOM  3178 OE1 GLU B 151     20.307  78.389  33.362  1.00 33.36      B   O
ATOM  3179 OE2 GLU B 151     21.204  78.716  31.378  1.00 24.62      B   O
ATOM  3180 C   GLU B 151     18.695  83.293  32.436  1.00 15.49      B   C
ATOM  3181 O   GLU B 151     19.515  83.243  31.522  1.00 16.76      B   O
ATOM  3182 N   SER B 152     17.746  84.218  32.514  1.00 15.83      B   N
ATOM  3183 CA  SER B 152     17.591  85.277  31.523  1.00 16.90      B   C
ATOM  3184 CB  SER B 152     18.843  86.159  31.486  1.00 16.89      B   C
ATOM  3185 OG  SER B 152     18.547  87.404  30.872  1.00 19.93      B   O
ATOM  3186 C   SER B 152     17.274  84.786  30.108  1.00 15.72      B   C
ATOM  3187 O   SER B 152     17.776  85.339  29.128  1.00 16.57      B   O
ATOM  3188 N   ILE B 153     16.452  83.746  30.003  1.00 16.59      B   N
ATOM  3189 CA  ILE B 153     16.048  83.223  28.701  1.00 16.23      B   C
ATOM  3190 CB  ILE B 153     15.840  81.688  28.747  1.00 17.80      B   C
ATOM  3191 CG2 ILE B 153     15.479  81.164  27.366  1.00 16.97      B   C
ATOM  3192 CG1 ILE B 153     17.118  81.008  29.247  1.00 18.17      B   C
ATOM  3193 CD1 ILE B 153     18.328  81.264  28.379  1.00 20.45      B   C
ATOM  3194 C   ILE B 153     14.716  83.924  28.465  1.00 17.00      B   C
ATOM  3195 O   ILE B 153     13.647  83.337  28.649  1.00 16.86      B   O
ATOM  3196 N   LEU B 154     14.802  85.192  28.074  1.00 16.13      B   N
ATOM  3197 CA  LEU B 154     13.629  86.036  27.861  1.00 17.93      B   C
ATOM  3198 CB  LEU B 154     13.891  87.412  28.475  1.00 15.30      B   C
ATOM  3199 CG  LEU B 154     14.390  87.335  29.923  1.00 14.99      B   C
ATOM  3200 CD1 LEU B 154     14.685  88.728  30.459  1.00 17.09      B   C
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Figure 5EEE

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ATOM  3201 CD2 LEU B 154    13.348  86.640  30.776  1.00 18.19    B   C
ATOM  3202 C   LEU B 154    13.188  86.204  26.413  1.00 19.02    B   C
ATOM  3203 O   LEU B 154    12.258  86.956  26.125  1.00 18.98    B   O
ATOM  3204 N   GLU B 155    13.857  85.506  25.506  1.00 19.46    B   N
ATOM  3205 CA  GLU B 155    13.520  85.579  24.093  1.00 20.61    B   C
ATOM  3206 CB  GLU B 155    14.055  86.877  23.481  1.00 23.20    B   C
ATOM  3207 CG  GLU B 155    15.563  86.894  23.285  1.00 31.50    B   C
ATOM  3208 CD  GLU B 155    16.077  88.235  22.778  1.00 39.23    B   C
ATOM  3209 OE1 GLU B 155    15.483  88.786  21.824  1.00 42.91    B   O
ATOM  3210 OE2 GLU B 155    17.084  88.734  23.328  1.00 43.36    B   O
ATOM  3211 C   GLU B 155    14.177  84.391  23.421  1.00 19.99    B   C
ATOM  3212 O   GLU B 155    14.864  83.610  24.077  1.00 21.64    B   O
ATOM  3213 N   GLY B 156    13.946  84.242  22.121  1.00 20.12    B   N
ATOM  3214 CA  GLY B 156    14.563  83.152  21.396  1.00 19.17    B   C
ATOM  3215 C   GLY B 156    13.844  81.820  21.366  1.00 20.79    B   C
ATOM  3216 O   GLY B 156    12.804  81.618  21.995  1.00 18.13    B   O
ATOM  3217 N   GLU B 157    14.451  80.898  20.626  1.00 22.19    B   N
ATOM  3218 CA  GLU B 157    13.946  79.548  20.415  1.00 21.56    B   C
ATOM  3219 CB  GLU B 157    14.952  78.782  19.553  1.00 25.02    B   C
ATOM  3220 CG  GLU B 157    14.524  77.377  19.184  1.00 35.87    B   C
ATOM  3221 CD  GLU B 157    15.499  76.703  18.231  1.00 41.09    B   C
ATOM  3222 OE1 GLU B 157    16.701  76.596  18.573  1.00 42.82    B   O
ATOM  3223 OE2 GLU B 157    15.058  76.275  17.141  1.00 42.70    B   O
ATOM  3224 C   GLU B 157    13.613  78.732  21.666  1.00 20.08    B   C
ATOM  3225 O   GLU B 157    12.588  78.044  21.702  1.00 18.27    B   O
ATOM  3226 N   LEU B 158    14.471  78.796  22.683  1.00 17.09    B   N
ATOM  3227 CA  LEU B 158    14.238  78.033  23.904  1.00 15.87    B   C
ATOM  3228 CB  LEU B 158    15.447  78.132  24.842  1.00 18.05    B   C
ATOM  3229 CG  LEU B 158    15.334  77.315  26.136  1.00 17.16    B   C
ATOM  3230 CD1 LEU B 158    14.977  75.872  25.807  1.00 15.66    B   C
ATOM  3231 CD2 LEU B 158    16.651  77.382  26.905  1.00 17.03    B   C
ATOM  3232 C   LEU B 158    12.973  78.488  24.630  1.00 16.52    B   C
ATOM  3233 O   LEU B 158    12.189  77.662  25.108  1.00 14.49    B   O
ATOM  3234 N   LEU B 159    12.775  79.799  24.727  1.00 14.92    B   N
ATOM  3235 CA  LEU B 159    11.580  80.306  25.383  1.00 14.51    B   C
ATOM  3236 CB  LEU B 159    11.660  81.823  25.578  1.00 15.13    B   C
ATOM  3237 CG  LEU B 159    10.374  82.456  26.133  1.00 16.38    B   C
ATOM  3238 CD1 LEU B 159     9.996  81.799  27.450  1.00 14.88    B   C
ATOM  3239 CD2 LEU B 159    10.574  83.955  26.326  1.00 15.09    B   C
ATOM  3240 C   LEU B 159    10.367  79.951  24.519  1.00 14.59    B   C
ATOM  3241 O   LEU B 159     9.350  79.492  25.028  1.00 13.56    B   O
ATOM  3242 N   GLU B 160    10.483  80.150  23.209  1.00 14.14    B   N
ATOM  3243 CA  GLU B 160     9.382  79.820  22.304  1.00 16.06    B   C
ATOM  3244 CB  GLU B 160     9.779  80.107  20.853  1.00 18.15    B   C
ATOM  3245 CG  GLU B 160     8.709  79.743  19.815  1.00 23.84    B   C
ATOM  3246 CD  GLU B 160     7.357  80.384  20.107  1.00 27.35    B   C
ATOM  3247 OE1 GLU B 160     7.330  81.496  20.683  1.00 24.13    B   O
ATOM  3248 OE2 GLU B 160     6.321  79.783  19.748  1.00 30.37    B   O
ATOM  3249 C   GLU B 160     8.987  78.348  22.438  1.00 15.10    B   C
ATOM  3250 O   GLU B 160     7.811  78.015  22.566  1.00 16.67    B   O
ATOM  3251 N   THR B 161     9.979  77.469  22.416  1.00 15.36    B   N
ATOM  3252 CA  THR B 161     9.720  76.037  22.518  1.00 16.10    B   C
ATOM  3253 CB  THR B 161    11.024  75.243  22.343  1.00 17.81    B   C
ATOM  3254 OG1 THR B 161    11.607  75.567  21.072  1.00 19.62    B   O
ATOM  3255 CG2 THR B 161    10.756  73.748  22.407  1.00 18.12    B   C
ATOM  3256 C   THR B 161     9.066  75.676  23.851  1.00 14.89    B   C
ATOM  3257 O   THR B 161     8.172  74.821  23.907  1.00 13.07    B   O
ATOM  3258 N   CYS B 162     9.500  76.342  24.918  1.00 12.65    B   N
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Figure 5FFF

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ATOM  3259 CA  CYS B 162     8.958  76.087  26.248  1.00 15.38    B   C
ATOM  3260 CB  CYS B 162     9.800  76.796  27.310  1.00 14.79    B   C
ATOM  3261 SG  CYS B 162     9.400  76.328  29.021  1.00 16.89    B   S
ATOM  3262 C   CYS B 162     7.505  76.557  26.341  1.00 15.60    B   C
ATOM  3263 O   CYS B 162     6.651  75.849  26.877  1.00 15.21    B   O
ATOM  3264 N   MET B 163     7.226  77.756  25.831  1.00 15.17    B   N
ATOM  3265 CA  MET B 163     5.863  78.271  25.860  1.00 15.78    B   C
ATOM  3266 CB  MET B 163     5.792  79.695  25.294  1.00 15.75    B   C
ATOM  3267 CG  MET B 163     6.424  80.767  26.162  1.00 16.77    B   C
ATOM  3268 SD  MET B 163     5.978  82.432  25.603  1.00 16.61    B   S
ATOM  3269 CE  MET B 163     6.937  82.509  24.114  1.00 14.38    B   C
ATOM  3270 C   MET B 163     4.962  77.360  25.033  1.00 14.99    B   C
ATOM  3271 O   MET B 163     3.819  77.093  25.410  1.00 15.77    B   O
ATOM  3272 N   HIS B 164     5.484  76.879  23.909  1.00 15.34    B   N
ATOM  3273 CA  HIS B 164     4.718  76.002  23.033  1.00 19.25    B   C
ATOM  3274 CB  HIS B 164     5.504  75.724  21.751  1.00 20.62    B   C
ATOM  3275 CG  HIS B 164     4.693  75.055  20.688  1.00 28.25    B   C
ATOM  3276 CD2 HIS B 164     4.779  73.817  20.146  1.00 28.01    B   C
ATOM  3277 ND1 HIS B 164     3.608  75.661  20.090  1.00 29.20    B   N
ATOM  3278 CE1 HIS B 164     3.060  74.824  19.227  1.00 29.23    B   C
ATOM  3279 NE2 HIS B 164     3.750  73.698  19.243  1.00 29.55    B   N
ATOM  3280 C   HIS B 164     4.412  74.690  23.760  1.00 19.47    B   C
ATOM  3281 O   HIS B 164     3.293  74.169  23.704  1.00 17.49    B   O
ATOM  3282 N   TYR B 165     5.419  74.169  24.449  1.00 17.68    B   N
ATOM  3283 CA  TYR B 165     5.277  72.937  25.210  1.00 16.69    B   C
ATOM  3284 CB  TYR B 165     6.578  72.655  25.969  1.00 15.68    B   C
ATOM  3285 CG  TYR B 165     6.457  71.544  26.976  1.00 17.57    B   C
ATOM  3286 CD1 TYR B 165     6.384  70.211  26.569  1.00 16.95    B   C
ATOM  3287 CE1 TYR B 165     6.216  69.191  27.498  1.00 20.45    B   C
ATOM  3288 CD2 TYR B 165     6.362  71.829  28.336  1.00 15.75    B   C
ATOM  3289 CE2 TYR B 165     6.193  70.818  29.273  1.00 17.81    B   C
ATOM  3290 CZ  TYR B 165     6.119  69.501  28.847  1.00 18.80    B   C
ATOM  3291 OH  TYR B 165     5.941  68.500  29.773  1.00 19.07    B   O
ATOM  3292 C   TYR B 165     4.101  73.027  26.193  1.00 16.83    B   C
ATOM  3293 O   TYR B 165     3.303  72.094  26.310  1.00 19.76    B   O
ATOM  3294 N   TYR B 166     3.999  74.151  26.895  1.00 16.40    B   N
ATOM  3295 CA  TYR B 166     2.931  74.369  27.864  1.00 16.70    B   C
ATOM  3296 CB  TYR B 166     3.362  75.435  28.888  1.00 13.68    B   C
ATOM  3297 CG  TYR B 166     4.354  74.961  29.930  1.00 15.63    B   C
ATOM  3298 CD1 TYR B 166     5.545  75.650  30.150  1.00 13.48    B   C
ATOM  3299 CE1 TYR B 166     6.458  75.218  31.113  1.00 17.41    B   C
ATOM  3300 CD2 TYR B 166     4.097  73.825  30.702  1.00 16.97    B   C
ATOM  3301 CE2 TYR B 166     5.001  73.387  31.668  1.00 14.41    B   C
ATOM  3302 CZ  TYR B 166     6.176  74.084  31.868  1.00 15.99    B   C
ATOM  3303 OH  TYR B 166     7.058  73.648  32.827  1.00 15.83    B   O
ATOM  3304 C   TYR B 166     1.576  74.793  27.278  1.00 17.53    B   C
ATOM  3305 O   TYR B 166     0.529  74.344  27.746  1.00 18.77    B   O
ATOM  3306 N   PHE B 167     1.599  75.651  26.260  1.00 18.80    B   N
ATOM  3307 CA  PHE B 167     0.367  76.198  25.668  1.00 19.74    B   C
ATOM  3308 CB  PHE B 167     0.660  77.589  25.115  1.00 18.42    B   C
ATOM  3309 CG  PHE B 167     1.092  78.573  26.163  1.00 17.20    B   C
ATOM  3310 CD1 PHE B 167     1.928  79.627  25.824  1.00 16.80    B   C
ATOM  3311 CD2 PHE B 167     0.635  78.472  27.482  1.00 16.87    B   C
ATOM  3312 CE1 PHE B 167     2.306  80.572  26.770  1.00 17.05    B   C
ATOM  3313 CE2 PHE B 167     1.010  79.419  28.439  1.00 17.71    B   C
ATOM  3314 CZ  PHE B 167     1.851  80.472  28.075  1.00 17.51    B   C
ATOM  3315 C   PHE B 167    -0.367  75.383  24.618  1.00 21.10    B   C
ATOM  3316 O   PHE B 167    -1.597  75.430  24.535  1.00 19.22    B   O
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Figure 5GGG

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ATOM  3317  N   THR B 168      0.403  74.657  23.812  1.00 23.27    B   N
ATOM  3318  CA  THR B 168     -0.165  73.805  22.765  1.00 26.77    B   C
ATOM  3319  CB  THR B 168      0.865  72.832  22.187  1.00 27.57    B   C
ATOM  3320  OG1 THR B 168      1.911  73.535  21.517  1.00 32.03    B   O
ATOM  3321  CG2 THR B 168      0.186  71.880  21.180  1.00 32.54    B   C
ATOM  3322  C   THR B 168     -1.363  72.944  23.205  1.00 26.77    B   C
ATOM  3323  O   THR B 168     -2.395  72.938  22.572  1.00 28.26    B   O
ATOM  3324  N   PRO B 169     -1.239  72.197  24.326  1.00 26.46    B   N
ATOM  3325  CD  PRO B 169     -0.050  72.083  25.152  1.00 26.67    B   C
ATOM  3326  CA  PRO B 169     -2.291  71.326  24.883  1.00 25.55    B   C
ATOM  3327  CB  PRO B 169     -1.610  70.668  26.066  1.00 26.50    B   C
ATOM  3328  CG  PRO B 169     -0.169  70.666  25.699  1.00 26.43    B   C
ATOM  3329  C   PRO B 169     -3.593  72.077  25.297  1.00 24.82    B   C
ATOM  3330  O   PRO B 169     -4.610  71.418  25.576  1.00 24.34    B   O
ATOM  3331  N   LEU B 170     -3.536  73.405  25.391  1.00 22.80    B   N
ATOM  3332  CA  LEU B 170     -4.729  74.167  25.761  1.00 25.50    B   C
ATOM  3333  CB  LEU B 170     -4.385  75.632  25.964  1.00 23.84    B   C
ATOM  3334  CG  LEU B 170     -3.514  75.982  27.186  1.00 25.53    B   C
ATOM  3335  CD1 LEU B 170     -3.138  77.463  27.146  1.00 26.01    B   C
ATOM  3336  CD2 LEU B 170     -4.242  75.652  28.503  1.00 26.09    B   C
ATOM  3337  C   LEU B 170     -5.772  74.057  24.644  1.00 25.77    B   C
ATOM  3338  O   LEU B 170     -5.436  74.103  23.453  1.00 26.97    B   O
ATOM  3339  N   GLU B 171     -7.033  73.952  25.037  1.00 27.92    B   N
ATOM  3340  CA  GLU B 171     -8.117  73.860  24.078  1.00 30.46    B   C
ATOM  3341  CB  GLU B 171     -9.035  72.693  24.435  1.00 34.23    B   C
ATOM  3342  CG  GLU B 171     -8.408  71.310  24.268  1.00 36.53    B   C
ATOM  3343  CD  GLU B 171     -7.963  71.029  22.844  1.00 38.06    B   C
ATOM  3344  OE1 GLU B 171     -8.773  71.218  21.911  1.00 38.60    B   O
ATOM  3345  OE2 GLU B 171     -6.800  70.614  22.659  1.00 38.27    B   O
ATOM  3346  C   GLU B 171     -8.903  75.155  24.104  1.00 30.56    B   C
ATOM  3347  O   GLU B 171     -9.477  75.560  23.093  1.00 33.13    B   O
ATOM  3348  N   ILE B 172     -8.922  75.801  25.265  1.00 27.64    B   N
ATOM  3349  CA  ILE B 172     -9.627  77.060  25.428  1.00 26.46    B   C
ATOM  3350  CB  ILE B 172    -10.239  77.179  26.838  1.00 26.68    B   C
ATOM  3351  CG2 ILE B 172    -10.916  78.534  26.994  1.00 26.23    B   C
ATOM  3352  CG1 ILE B 172    -11.246  76.050  27.071  1.00 27.08    B   C
ATOM  3353  CD1 ILE B 172    -11.899  76.085  28.443  1.00 27.76    B   C
ATOM  3354  C   ILE B 172     -8.670  78.225  25.218  1.00 26.74    B   C
ATOM  3355  O   ILE B 172     -7.604  78.284  25.833  1.00 24.89    B   O
ATOM  3356  N   LEU B 173     -9.055  79.148  24.343  1.00 25.65    B   N
ATOM  3357  CA  LEU B 173     -8.245  80.328  24.061  1.00 25.77    B   C
ATOM  3358  CB  LEU B 173     -8.564  80.853  22.659  1.00 28.20    B   C
ATOM  3359  CG  LEU B 173     -7.682  81.962  22.082  1.00 29.17    B   C
ATOM  3360  CD1 LEU B 173     -6.227  81.521  22.081  1.00 31.35    B   C
ATOM  3361  CD2 LEU B 173     -8.144  82.281  20.661  1.00 29.98    B   C
ATOM  3362  C   LEU B 173     -8.585  81.387  25.111  1.00 24.69    B   C
ATOM  3363  O   LEU B 173     -9.720  81.852  25.188  1.00 26.80    B   O
ATOM  3364  N   PRO B 174     -7.606  81.780  25.939  1.00 21.86    B   N
ATOM  3365  CD  PRO B 174     -6.227  81.269  26.032  1.00 20.12    B   C
ATOM  3366  CA  PRO B 174     -7.857  82.786  26.973  1.00 21.00    B   C
ATOM  3367  CB  PRO B 174     -6.629  82.663  27.873  1.00 20.86    B   C
ATOM  3368  CG  PRO B 174     -5.553  82.313  26.900  1.00 20.88    B   C
ATOM  3369  C   PRO B 174     -8.058  84.215  26.481  1.00 21.07    B   C
ATOM  3370  O   PRO B 174     -7.442  84.652  25.510  1.00 20.92    B   O
ATOM  3371  N   GLU B 175     -8.941  84.932  27.163  1.00 20.88    B   N
ATOM  3372  CA  GLU B 175     -9.210  86.325  26.849  1.00 20.49    B   C
ATOM  3373  CB  GLU B 175     -10.714  86.599  26.886  1.00 22.18    B   C
ATOM  3374  CG  GLU B 175     -11.414  86.262  25.584  1.00 24.72    B   C
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Figure 5HHH

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ATOM  3375 CD  GLU B 175    -12.914  86.445  25.662  1.00 27.87    B   C
ATOM  3376 OE1 GLU B 175    -13.362  87.355  26.386  1.00 29.73    B   O
ATOM  3377 OE2 GLU B 175    -13.643  85.686  24.989  1.00 30.38    B   O
ATOM  3378 C   GLU B 175     -8.492  87.110  27.932  1.00 19.76    B   C
ATOM  3379 O   GLU B 175     -8.151  88.278  27.760  1.00 19.06    B   O
ATOM  3380 N   VAL B 176     -8.249  86.429  29.047  1.00 18.72    B   N
ATOM  3381 CA  VAL B 176     -7.561  87.013  30.187  1.00 18.26    B   C
ATOM  3382 CB  VAL B 176     -8.542  87.366  31.329  1.00 19.04    B   C
ATOM  3383 CG1 VAL B 176     -7.792  88.005  32.473  1.00 17.96    B   C
ATOM  3384 CG2 VAL B 176     -9.627  88.307  30.819  1.00 19.77    B   C
ATOM  3385 C   VAL B 176     -6.566  85.994  30.728  1.00 18.77    B   C
ATOM  3386 O   VAL B 176     -6.909  84.830  30.936  1.00 18.44    B   O
ATOM  3387 N   ILE B 177     -5.337  86.438  30.955  1.00 15.78    B   N
ATOM  3388 CA  ILE B 177     -4.302  85.564  31.485  1.00 15.67    B   C
ATOM  3389 CB  ILE B 177     -3.149  85.366  30.479  1.00 16.57    B   C
ATOM  3390 CG2 ILE B 177     -2.076  84.471  31.092  1.00 15.73    B   C
ATOM  3391 CG1 ILE B 177     -3.679  84.754  29.184  1.00 17.67    B   C
ATOM  3392 CD1 ILE B 177     -2.639  84.634  28.094  1.00 16.12    B   C
ATOM  3393 C   ILE B 177     -3.730  86.191  32.746  1.00 15.83    B   C
ATOM  3394 O   ILE B 177     -3.319  87.356  32.742  1.00 15.47    B   O
ATOM  3395 N   ILE B 178     -3.721  85.427  33.832  1.00 15.84    B   N
ATOM  3396 CA  ILE B 178     -3.178  85.932  35.080  1.00 15.63    B   C
ATOM  3397 CB  ILE B 178     -3.958  85.402  36.314  1.00 16.93    B   C
ATOM  3398 CG2 ILE B 178     -3.370  85.986  37.589  1.00 15.87    B   C
ATOM  3399 CG1 ILE B 178     -5.432  85.807  36.228  1.00 18.02    B   C
ATOM  3400 CD1 ILE B 178     -6.267  85.341  37.422  1.00 17.46    B   C
ATOM  3401 C   ILE B 178     -1.724  85.486  35.190  1.00 14.02    B   C
ATOM  3402 O   ILE B 178     -1.416  84.300  35.089  1.00 13.65    B   O
ATOM  3403 N   LEU B 179     -0.833  86.449  35.376  1.00 14.12    B   N
ATOM  3404 CA  LEU B 179      0.589  86.150  35.525  1.00 14.34    B   C
ATOM  3405 CB  LEU B 179      1.428  87.340  35.053  1.00 15.34    B   C
ATOM  3406 CG  LEU B 179      1.169  87.783  33.610  1.00 16.04    B   C
ATOM  3407 CD1 LEU B 179      1.942  89.073  33.332  1.00 18.24    B   C
ATOM  3408 CD2 LEU B 179      1.574  86.680  32.636  1.00 16.26    B   C
ATOM  3409 C   LEU B 179      0.783  85.915  37.021  1.00 14.01    B   C
ATOM  3410 O   LEU B 179      1.391  86.727  37.719  1.00 13.42    B   O
ATOM  3411 N   GLY B 180      0.252  84.790  37.493  1.00 13.50    B   N
ATOM  3412 CA  GLY B 180      0.310  84.448  38.906  1.00 13.79    B   C
ATOM  3413 C   GLY B 180      1.632  83.927  39.417  1.00 12.30    B   C
ATOM  3414 O   GLY B 180      1.681  82.902  40.093  1.00 14.02    B   O
ATOM  3415 N   CYS B 181      2.702  84.647  39.093  1.00 13.12    B   N
ATOM  3416 CA  CYS B 181      4.048  84.295  39.518  1.00 11.26    B   C
ATOM  3417 CB  CYS B 181      4.591  83.150  38.667  1.00 11.52    B   C
ATOM  3418 SG  CYS B 181      6.279  82.671  39.091  1.00 14.29    B   S
ATOM  3419 C   CYS B 181      4.927  85.532  39.348  1.00 11.67    B   C
ATOM  3420 O   CYS B 181      4.837  86.226  38.336  1.00 10.15    B   O
ATOM  3421 N   THR B 182      5.770  85.796  40.342  1.00 10.95    B   N
ATOM  3422 CA  THR B 182      6.671  86.950  40.329  1.00 11.68    B   C
ATOM  3423 CB  THR B 182      7.654  86.902  41.517  1.00 12.29    B   C
ATOM  3424 OG1 THR B 182      8.306  85.623  41.546  1.00  8.82    B   O
ATOM  3425 CG2 THR B 182      6.918  87.133  42.832  1.00 13.05    B   C
ATOM  3426 C   THR B 182      7.511  87.085  39.068  1.00 12.00    B   C
ATOM  3427 O   THR B 182      7.775  88.190  38.604  1.00 11.14    B   O
ATOM  3428 N   HIS B 183      7.927  85.953  38.516  1.00 11.51    B   N
ATOM  3429 CA  HIS B 183      8.782  85.934  37.333  1.00 12.53    B   C
ATOM  3430 CB  HIS B 183      9.490  84.577  37.250  1.00 12.11    B   C
ATOM  3431 CG  HIS B 183     10.413  84.301  38.396  1.00 12.62    B   C
ATOM  3432 CD2 HIS B 183     11.662  83.774  38.425  1.00 14.37    B   C
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Figure 5III

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ATOM  3433 ND1 HIS B 183    10.074  84.558  39.708  1.00 12.87    B   N
ATOM  3434 CE1 HIS B 183    11.076  84.206  40.495  1.00 11.92    B   C
ATOM  3435 NE2 HIS B 183    12.051  83.728  39.741  1.00 12.64    B   N
ATOM  3436 C   HIS B 183     8.113  86.202  35.990  1.00 13.70    B   C
ATOM  3437 O   HIS B 183     8.735  86.757  35.082  1.00 14.63    B   O
ATOM  3438 N   PHE B 184     6.846  85.822  35.866  1.00 14.67    B   N
ATOM  3439 CA  PHE B 184     6.134  85.945  34.595  1.00 13.80    B   C
ATOM  3440 CB  PHE B 184     4.751  85.298  34.731  1.00 14.23    B   C
ATOM  3441 CG  PHE B 184     4.809  83.829  35.102  1.00 13.65    B   C
ATOM  3442 CD1 PHE B 184     3.646  83.084  35.240  1.00 16.74    B   C
ATOM  3443 CD2 PHE B 184     6.035  83.207  35.355  1.00 14.92    B   C
ATOM  3444 CE1 PHE B 184     3.698  81.743  35.631  1.00 13.35    B   C
ATOM  3445 CE2 PHE B 184     6.097  81.866  35.746  1.00 14.40    B   C
ATOM  3446 CZ  PHE B 184     4.923  81.136  35.884  1.00 13.35    B   C
ATOM  3447 C   PHE B 184     6.049  87.314  33.921  1.00 13.82    B   C
ATOM  3448 O   PHE B 184     5.991  87.391  32.691  1.00 13.30    B   O
ATOM  3449 N   PRO B 185     6.032  88.409  34.697  1.00 13.55    B   N
ATOM  3450 CD  PRO B 185     5.786  88.577  36.143  1.00 14.61    B   C
ATOM  3451 CA  PRO B 185     5.966  89.701  34.008  1.00 14.00    B   C
ATOM  3452 CB  PRO B 185     5.964  90.702  35.158  1.00 15.55    B   C
ATOM  3453 CG  PRO B 185     5.186  89.971  36.210  1.00 16.68    B   C
ATOM  3454 C   PRO B 185     7.158  89.907  33.063  1.00 14.41    B   C
ATOM  3455 O   PRO B 185     7.057  90.640  32.076  1.00 14.66    B   O
ATOM  3456 N   LEU B 186     8.285  89.257  33.355  1.00 13.60    B   N
ATOM  3457 CA  LEU B 186     9.462  89.410  32.503  1.00 14.78    B   C
ATOM  3458 CB  LEU B 186    10.707  88.844  33.185  1.00 16.45    B   C
ATOM  3459 CG  LEU B 186    11.268  89.716  34.312  1.00 17.76    B   C
ATOM  3460 CD1 LEU B 186    12.601  89.149  34.788  1.00 18.57    B   C
ATOM  3461 CD2 LEU B 186    11.454  91.145  33.800  1.00 19.96    B   C
ATOM  3462 C   LEU B 186     9.299  88.796  31.115  1.00 14.26    B   C
ATOM  3463 O   LEU B 186    10.105  89.060  30.219  1.00 13.67    B   O
ATOM  3464 N   ILE B 187     8.271  87.973  30.933  1.00 13.72    B   N
ATOM  3465 CA  ILE B 187     8.007  87.391  29.616  1.00 14.52    B   C
ATOM  3466 CB  ILE B 187     8.252  85.852  29.567  1.00 16.13    B   C
ATOM  3467 CG2 ILE B 187     9.734  85.563  29.730  1.00 15.11    B   C
ATOM  3468 CG1 ILE B 187     7.418  85.134  30.630  1.00 14.95    B   C
ATOM  3469 CD1 ILE B 187     7.386  83.616  30.452  1.00 18.91    B   C
ATOM  3470 C   ILE B 187     6.559  87.681  29.216  1.00 15.97    B   C
ATOM  3471 O   ILE B 187     5.970  86.973  28.399  1.00 14.41    B   O
ATOM  3472 N   ALA B 188     6.003  88.742  29.790  1.00 14.30    B   N
ATOM  3473 CA  ALA B 188     4.623  89.138  29.511  1.00 16.72    B   C
ATOM  3474 CB  ALA B 188     4.261  90.381  30.318  1.00 17.73    B   C
ATOM  3475 C   ALA B 188     4.386  89.386  28.021  1.00 17.75    B   C
ATOM  3476 O   ALA B 188     3.473  88.806  27.437  1.00 15.55    B   O
ATOM  3477 N   GLN B 189     5.208  90.232  27.404  1.00 18.64    B   N
ATOM  3478 CA  GLN B 189     5.045  90.521  25.979  1.00 20.60    B   C
ATOM  3479 CB  GLN B 189     5.977  91.668  25.553  1.00 24.25    B   C
ATOM  3480 CG  GLN B 189     7.448  91.297  25.369  1.00 34.75    B   C
ATOM  3481 CD  GLN B 189     8.385  92.508  25.450  1.00 39.99    B   C
ATOM  3482 OE1 GLN B 189     7.963  93.653  25.263  1.00 43.74    B   O
ATOM  3483 NE2 GLN B 189     9.663  92.254  25.720  1.00 40.19    B   N
ATOM  3484 C   GLN B 189     5.279  89.273  25.111  1.00 17.97    B   C
ATOM  3485 O   GLN B 189     4.729  89.163  24.015  1.00 14.32    B   O
ATOM  3486 N   LYS B 190     6.078  88.329  25.606  1.00 17.40    B   N
ATOM  3487 CA  LYS B 190     6.341  87.097  24.859  1.00 16.80    B   C
ATOM  3488 CB  LYS B 190     7.567  86.374  25.421  1.00 18.22    B   C
ATOM  3489 CG  LYS B 190     8.878  87.117  25.218  1.00 21.88    B   C
ATOM  3490 CD  LYS B 190     9.211  87.269  23.740  1.00 25.45    B   C
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Figure 5JJJ

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ATOM  3491  CE  LYS B 190     10.416  88.179  23.543  1.00 29.36      B   C
ATOM  3492  NZ  LYS B 190     10.790  88.298  22.110  1.00 29.28      B   N
ATOM  3493  C   LYS B 190      5.123  86.176  24.920  1.00 16.76      B   C
ATOM  3494  O   LYS B 190      4.775  85.521  23.934  1.00 15.72      B   O
ATOM  3495  N   ILE B 191      4.484  86.118  26.085  1.00 17.36      B   N
ATOM  3496  CA  ILE B 191      3.293  85.293  26.250  1.00 16.65      B   C
ATOM  3497  CB  ILE B 191      2.835  85.283  27.722  1.00 16.29      B   C
ATOM  3498  CG2 ILE B 191      1.429  84.706  27.837  1.00 15.90      B   C
ATOM  3499  CG1 ILE B 191      3.827  84.472  28.561  1.00 14.41      B   C
ATOM  3500  CD1 ILE B 191      3.575  84.556  30.065  1.00 15.15      B   C
ATOM  3501  C   ILE B 191      2.206  85.902  25.371  1.00 17.73      B   C
ATOM  3502  O   ILE B 191      1.431  85.201  24.730  1.00 17.39      B   O
ATOM  3503  N   GLU B 192      2.174  87.227  25.343  1.00 19.90      B   N
ATOM  3504  CA  GLU B 192      1.206  87.955  24.545  1.00 20.35      B   C
ATOM  3505  CB  GLU B 192      1.368  89.452  24.811  1.00 22.52      B   C
ATOM  3506  CG  GLU B 192      0.186  90.301  24.426  1.00 31.49      B   C
ATOM  3507  CD  GLU B 192      0.310  91.705  24.981  1.00 36.51      B   C
ATOM  3508  OE1 GLU B 192      0.342  91.845  26.223  1.00 39.33      B   O
ATOM  3509  OE2 GLU B 192      0.384  92.660  24.179  1.00 38.77      B   O
ATOM  3510  C   GLU B 192      1.468  87.638  23.077  1.00 18.85      B   C
ATOM  3511  O   GLU B 192      0.553  87.274  22.327  1.00 18.00      B   O
ATOM  3512  N   GLY B 193      2.733  87.764  22.685  1.00 19.26      B   N
ATOM  3513  CA  GLY B 193      3.134  87.497  21.319  1.00 16.37      B   C
ATOM  3514  C   GLY B 193      2.843  86.078  20.880  1.00 17.40      B   C
ATOM  3515  O   GLY B 193      2.580  85.832  19.700  1.00 19.53      B   O
ATOM  3516  N   TYR B 194      2.892  85.138  21.819  1.00 15.60      B   N
ATOM  3517  CA  TYR B 194      2.621  83.740  21.494  1.00 16.39      B   C
ATOM  3518  CB  TYR B 194      2.829  82.845  22.715  1.00 16.47      B   C
ATOM  3519  CG  TYR B 194      2.502  81.386  22.452  1.00 15.75      B   C
ATOM  3520  CD1 TYR B 194      3.470  80.515  21.964  1.00 17.79      B   C
ATOM  3521  CE1 TYR B 194      3.171  79.178  21.698  1.00 18.26      B   C
ATOM  3522  CD2 TYR B 194      1.216  80.887  22.669  1.00 15.15      B   C
ATOM  3523  CE2 TYR B 194      0.904  79.551  22.403  1.00 16.44      B   C
ATOM  3524  CZ  TYR B 194      1.890  78.703  21.920  1.00 15.60      B   C
ATOM  3525  OH  TYR B 194      1.614  77.379  21.671  1.00 17.72      B   O
ATOM  3526  C   TYR B 194      1.189  83.551  21.003  1.00 16.01      B   C
ATOM  3527  O   TYR B 194      0.966  82.985  19.940  1.00 17.33      B   O
ATOM  3528  N   PHE B 195      0.218  84.011  21.785  1.00 17.37      B   N
ATOM  3529  CA  PHE B 195     -1.177  83.851  21.390  1.00 19.84      B   C
ATOM  3530  CB  PHE B 195     -2.108  84.174  22.563  1.00 20.48      B   C
ATOM  3531  CG  PHE B 195     -2.057  83.146  23.659  1.00 21.18      B   C
ATOM  3532  CD1 PHE B 195     -1.166  83.281  24.720  1.00 20.24      B   C
ATOM  3533  CD2 PHE B 195     -2.847  82.002  23.590  1.00 20.40      B   C
ATOM  3534  CE1 PHE B 195     -1.061  82.289  25.692  1.00 18.52      B   C
ATOM  3535  CE2 PHE B 195     -2.748  81.004  24.558  1.00 21.83      B   C
ATOM  3536  CZ  PHE B 195     -1.853  81.149  25.609  1.00 18.80      B   C
ATOM  3537  C   PHE B 195     -1.549  84.675  20.168  1.00 21.22      B   C
ATOM  3538  O   PHE B 195     -2.381  84.260  19.364  1.00 23.42      B   O
ATOM  3539  N   MET B 196     -0.920  85.835  20.018  1.00 20.91      B   N
ATOM  3540  CA  MET B 196     -1.191  86.691  18.874  1.00 22.63      B   C
ATOM  3541  CB  MET B 196     -0.632  88.096  19.110  1.00 21.19      B   C
ATOM  3542  CG  MET B 196     -1.454  88.939  20.066  1.00 21.47      B   C
ATOM  3543  SD  MET B 196     -3.106  89.333  19.420  1.00 22.89      B   S
ATOM  3544  CE  MET B 196     -2.734  90.738  18.369  1.00 25.90      B   C
ATOM  3545  C   MET B 196     -0.574  86.098  17.616  1.00 22.76      B   C
ATOM  3546  O   MET B 196     -1.034  86.365  16.510  1.00 22.32      B   O
ATOM  3547  N   GLY B 197      0.462  85.284  17.788  1.00 23.35      B   N
ATOM  3548  CA  GLY B 197      1.117  84.682  16.644  1.00 23.78      B   C
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Figure 5KKK

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ATOM  3549  C   GLY B 197     0.612  83.294  16.308  1.00 26.07    B   C
ATOM  3550  O   GLY B 197     0.757  82.836  15.178  1.00 27.06    B   O
ATOM  3551  N   HIS B 198     0.011  82.618  17.280  1.00 24.62    B   N
ATOM  3552  CA  HIS B 198    -0.489  81.270  17.052  1.00 25.26    B   C
ATOM  3553  CB  HIS B 198    -0.143  80.393  18.250  1.00 24.79    B   C
ATOM  3554  CG  HIS B 198     1.318  80.087  18.358  1.00 27.65    B   C
ATOM  3555  CD2 HIS B 198     2.369  80.867  18.706  1.00 27.06    B   C
ATOM  3556  ND1 HIS B 198     1.847  78.858  18.026  1.00 29.54    B   N
ATOM  3557  CE1 HIS B 198     3.161  78.896  18.162  1.00 28.74    B   C
ATOM  3558  NE2 HIS B 198     3.503  80.104  18.572  1.00 27.31    B   N
ATOM  3559  C   HIS B 198    -1.982  81.189  16.742  1.00 25.16    B   C
ATOM  3560  O   HIS B 198    -2.470  80.160  16.274  1.00 25.84    B   O
ATOM  3561  N   PHE B 199    -2.701  82.274  17.002  1.00 23.99    B   N
ATOM  3562  CA  PHE B 199    -4.134  82.323  16.731  1.00 25.24    B   C
ATOM  3563  CB  PHE B 199    -4.939  82.150  18.021  1.00 25.35    B   C
ATOM  3564  CG  PHE B 199    -4.641  80.875  18.754  1.00 25.83    B   C
ATOM  3565  CD1 PHE B 199    -3.499  80.763  19.543  1.00 25.81    B   C
ATOM  3566  CD2 PHE B 199    -5.486  79.776  18.634  1.00 26.63    B   C
ATOM  3567  CE1 PHE B 199    -3.202  79.571  20.204  1.00 25.90    B   C
ATOM  3568  CE2 PHE B 199    -5.200  78.574  19.292  1.00 27.07    B   C
ATOM  3569  CZ  PHE B 199    -4.053  78.476  20.078  1.00 25.59    B   C
ATOM  3570  C   PHE B 199    -4.488  83.658  16.085  1.00 25.45    B   C
ATOM  3571  O   PHE B 199    -3.741  84.633  16.202  1.00 26.05    B   O
ATOM  3572  N   ALA B 200    -5.624  83.698  15.397  1.00 25.36    B   N
ATOM  3573  CA  ALA B 200    -6.066  84.926  14.744  1.00 26.49    B   C
ATOM  3574  CB  ALA B 200    -6.945  84.592  13.543  1.00 27.04    B   C
ATOM  3575  C   ALA B 200    -6.842  85.770  15.748  1.00 25.75    B   C
ATOM  3576  O   ALA B 200    -8.035  85.555  15.951  1.00 27.07    B   O
ATOM  3577  N   LEU B 201    -6.162  86.723  16.380  1.00 26.03    B   N
ATOM  3578  CA  LEU B 201    -6.801  87.588  17.371  1.00 25.45    B   C
ATOM  3579  CB  LEU B 201    -6.206  87.345  18.762  1.00 26.37    B   C
ATOM  3580  CG  LEU B 201    -6.409  85.971  19.404  1.00 27.87    B   C
ATOM  3581  CD1 LEU B 201    -5.727  85.944  20.768  1.00 27.55    B   C
ATOM  3582  CD2 LEU B 201    -7.895  85.681  19.539  1.00 28.11    B   C
ATOM  3583  C   LEU B 201    -6.668  89.069  17.041  1.00 24.86    B   C
ATOM  3584  O   LEU B 201    -5.571  89.565  16.801  1.00 25.77    B   O
ATOM  3585  N   PRO B 202    -7.792  89.795  17.036  1.00 25.07    B   N
ATOM  3586  CD  PRO B 202    -9.159  89.302  17.284  1.00 27.27    B   C
ATOM  3587  CA  PRO B 202    -7.801  91.229  16.739  1.00 27.30    B   C
ATOM  3588  CB  PRO B 202    -9.286  91.530  16.571  1.00 26.61    B   C
ATOM  3589  CG  PRO B 202    -9.919  90.581  17.541  1.00 28.74    B   C
ATOM  3590  C   PRO B 202    -7.162  92.024  17.878  1.00 28.85    B   C
ATOM  3591  O   PRO B 202    -6.625  93.111  17.676  1.00 31.54    B   O
ATOM  3592  N   THR B 203    -7.228  91.467  19.080  1.00 29.83    B   N
ATOM  3593  CA  THR B 203    -6.649  92.104  20.253  1.00 30.73    B   C
ATOM  3594  CB  THR B 203    -7.717  92.910  21.029  1.00 32.69    B   C
ATOM  3595  OG1 THR B 203    -7.113  93.535  22.168  1.00 38.76    B   O
ATOM  3596  CG2 THR B 203    -8.854  92.009  21.478  1.00 34.49    B   C
ATOM  3597  C   THR B 203    -6.057  91.009  21.142  1.00 30.11    B   C
ATOM  3598  O   THR B 203    -6.632  89.929  21.281  1.00 29.77    B   O
ATOM  3599  N   PRO B 204    -4.888  91.271  21.746  1.00 28.28    B   N
ATOM  3600  CD  PRO B 204    -4.105  92.519  21.714  1.00 29.99    B   C
ATOM  3601  CA  PRO B 204    -4.249  90.278  22.608  1.00 25.72    B   C
ATOM  3602  CB  PRO B 204    -2.871  90.878  22.851  1.00 27.64    B   C
ATOM  3603  CG  PRO B 204    -3.170  92.344  22.895  1.00 30.54    B   C
ATOM  3604  C   PRO B 204    -5.007  90.034  23.906  1.00 22.99    B   C
ATOM  3605  O   PRO B 204    -5.829  90.847  24.322  1.00 21.45    B   O
ATOM  3606  N   PRO B 205    -4.754  88.888  24.550  1.00 23.17    B   N
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Figure 5LLL

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ATOM  3607 CD  PRO B 205     -3.967  87.734  24.079  1.00 22.14    B   C
ATOM  3608 CA  PRO B 205     -5.435  88.579  25.812  1.00 21.71    B   C
ATOM  3609 CB  PRO B 205     -4.930  87.177  26.145  1.00 20.02    B   C
ATOM  3610 CG  PRO B 205     -4.640  86.587  24.791  1.00 24.28    B   C
ATOM  3611 C   PRO B 205     -5.013  89.592  26.870  1.00 20.42    B   C
ATOM  3612 O   PRO B 205     -3.884  90.081  26.855  1.00 20.68    B   O
ATOM  3613 N   LEU B 206     -5.920  89.912  27.781  1.00 19.56    B   N
ATOM  3614 CA  LEU B 206     -5.614  90.852  28.844  1.00 18.19    B   C
ATOM  3615 CB  LEU B 206     -6.903  91.341  29.506  1.00 19.98    B   C
ATOM  3616 CG  LEU B 206     -6.733  92.187  30.772  1.00 20.16    B   C
ATOM  3617 CD1 LEU B 206     -6.025  93.490  30.435  1.00 20.32    B   C
ATOM  3618 CD2 LEU B 206     -8.097  92.461  31.383  1.00 21.77    B   C
ATOM  3619 C   LEU B 206     -4.748  90.152  29.887  1.00 19.09    B   C
ATOM  3620 O   LEU B 206     -5.155  89.137  30.460  1.00 16.01    B   O
ATOM  3621 N   LEU B 207     -3.554  90.682  30.130  1.00 17.87    B   N
ATOM  3622 CA  LEU B 207     -2.673  90.086  31.128  1.00 19.96    B   C
ATOM  3623 CB  LEU B 207     -1.204  90.137  30.683  1.00 20.75    B   C
ATOM  3624 CG  LEU B 207     -0.775  89.375  29.427  1.00 23.64    B   C
ATOM  3625 CD1 LEU B 207      0.754  89.247  29.409  1.00 24.69    B   C
ATOM  3626 CD2 LEU B 207     -1.402  88.003  29.411  1.00 25.49    B   C
ATOM  3627 C   LEU B 207     -2.822  90.826  32.450  1.00 18.55    B   C
ATOM  3628 O   LEU B 207     -2.846  92.056  32.489  1.00 19.17    B   O
ATOM  3629 N   ILE B 208     -2.925  90.067  33.534  1.00 17.96    B   N
ATOM  3630 CA  ILE B 208     -3.064  90.645  34.860  1.00 17.50    B   C
ATOM  3631 CB  ILE B 208     -4.118  89.878  35.685  1.00 17.43    B   C
ATOM  3632 CG2 ILE B 208     -4.243  90.491  37.077  1.00 18.18    B   C
ATOM  3633 CG1 ILE B 208     -5.459  89.892  34.943  1.00 18.45    B   C
ATOM  3634 CD1 ILE B 208     -6.012  91.289  34.699  1.00 14.50    B   C
ATOM  3635 C   ILE B 208     -1.719  90.585  35.575  1.00 16.82    B   C
ATOM  3636 O   ILE B 208     -1.164  89.508  35.780  1.00 15.89    B   O
ATOM  3637 N   HIS B 209     -1.213  91.756  35.950  1.00 17.14    B   N
ATOM  3638 CA  HIS B 209      0.074  91.899  36.632  1.00 18.16    B   C
ATOM  3639 CB  HIS B 209      0.745  93.175  36.106  1.00 18.91    B   C
ATOM  3640 CG  HIS B 209      2.193  93.306  36.457  1.00 20.99    B   C
ATOM  3641 CD2 HIS B 209      3.306  93.162  35.699  1.00 19.36    B   C
ATOM  3642 ND1 HIS B 209      2.629  93.657  37.716  1.00 22.36    B   N
ATOM  3643 CE1 HIS B 209      3.949  93.725  37.718  1.00 21.52    B   C
ATOM  3644 NE2 HIS B 209      4.384  93.429  36.506  1.00 15.94    B   N
ATOM  3645 C   HIS B 209     -0.149  91.980  38.150  1.00 17.31    B   C
ATOM  3646 O   HIS B 209     -0.909  92.826  38.621  1.00 17.80    B   O
ATOM  3647 N   SER B 210      0.513  91.104  38.908  1.00 15.90    B   N
ATOM  3648 CA  SER B 210      0.361  91.070  40.366  1.00 18.09    B   C
ATOM  3649 CB  SER B 210      1.187  89.931  40.975  1.00 15.92    B   C
ATOM  3650 OG  SER B 210      0.783  88.671  40.475  1.00 17.30    B   O
ATOM  3651 C   SER B 210      0.762  92.368  41.048  1.00 18.89    B   C
ATOM  3652 O   SER B 210      0.146  92.783  42.036  1.00 18.64    B   O
ATOM  3653 N   GLY B 211      1.806  92.999  40.527  1.00 18.49    B   N
ATOM  3654 CA  GLY B 211      2.276  94.241  41.105  1.00 17.93    B   C
ATOM  3655 C   GLY B 211      1.300  95.384  40.929  1.00 18.65    B   C
ATOM  3656 O   GLY B 211      0.988  96.088  41.888  1.00 18.89    B   O
ATOM  3657 N   ASP B 212      0.821  95.585  39.708  1.00 17.89    B   N
ATOM  3658 CA  ASP B 212     -0.122  96.666  39.454  1.00 19.78    B   C
ATOM  3659 CB  ASP B 212     -0.441  96.776  37.959  1.00 21.36    B   C
ATOM  3660 CG  ASP B 212      0.789  97.074  37.119  1.00 25.55    B   C
ATOM  3661 OD1 ASP B 212      1.588  97.954  37.509  1.00 24.93    B   O
ATOM  3662 OD2 ASP B 212      0.948  96.432  36.059  1.00 27.71    B   O
ATOM  3663 C   ASP B 212     -1.414  96.441  40.227  1.00 18.76    B   C
ATOM  3664 O   ASP B 212     -2.025  97.389  40.712  1.00 19.27    B   O
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Figure 5MMM

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ATOM  3665 N   ALA B 213    -1.825  95.182  40.344  1.00 19.86    B   N
ATOM  3666 CA  ALA B 213    -3.055  94.847  41.054  1.00 17.54    B   C
ATOM  3667 CB  ALA B 213    -3.378  93.372  40.876  1.00 17.05    B   C
ATOM  3668 C   ALA B 213    -2.959  95.183  42.539  1.00 19.06    B   C
ATOM  3669 O   ALA B 213    -3.901  95.725  43.120  1.00 16.90    B   O
ATOM  3670 N   ILE B 214    -1.823  94.876  43.158  1.00 15.97    B   N
ATOM  3671 CA  ILE B 214    -1.678  95.162  44.577  1.00 16.41    B   C
ATOM  3672 CB  ILE B 214    -0.503  94.357  45.206  1.00 17.51    B   C
ATOM  3673 CG2 ILE B 214     0.841  94.960  44.809  1.00 16.99    B   C
ATOM  3674 CG1 ILE B 214    -0.639  94.359  46.733  1.00 17.48    B   C
ATOM  3675 CD1 ILE B 214     0.283  93.366  47.436  1.00 20.67    B   C
ATOM  3676 C   ILE B 214    -1.516  96.656  44.864  1.00 16.49    B   C
ATOM  3677 O   ILE B 214    -1.933  97.133  45.917  1.00 16.10    B   O
ATOM  3678 N   VAL B 215    -0.927  97.403  43.933  1.00 16.36    B   N
ATOM  3679 CA  VAL B 215    -0.772  98.841  44.139  1.00 17.16    B   C
ATOM  3680 CB  VAL B 215    -0.016  99.509  42.964  1.00 19.48    B   C
ATOM  3681 CG1 VAL B 215    -0.179 101.017  43.027  1.00 17.77    B   C
ATOM  3682 CG2 VAL B 215     1.470  99.147  43.022  1.00 17.10    B   C
ATOM  3683 C   VAL B 215    -2.161  99.471  44.259  1.00 18.05    B   C
ATOM  3684 O   VAL B 215    -2.417 100.282  45.153  1.00 17.39    B   O
ATOM  3685 N   GLU B 216    -3.054  99.089  43.354  1.00 19.67    B   N
ATOM  3686 CA  GLU B 216    -4.411  99.617  43.357  1.00 21.54    B   C
ATOM  3687 CB  GLU B 216    -5.188  99.059  42.166  1.00 23.84    B   C
ATOM  3688 CG  GLU B 216    -4.815  99.727  40.853  1.00 26.87    B   C
ATOM  3689 CD  GLU B 216    -5.388  99.014  39.648  1.00 30.91    B   C
ATOM  3690 OE1 GLU B 216    -5.399  99.623  38.558  1.00 34.30    B   O
ATOM  3691 OE2 GLU B 216    -5.815  97.845  39.785  1.00 31.99    B   O
ATOM  3692 C   GLU B 216    -5.126  99.293  44.657  1.00 20.92    B   C
ATOM  3693 O   GLU B 216    -5.815 100.141  45.223  1.00 19.64    B   O
ATOM  3694 N   TYR B 217    -4.955  98.065  45.135  1.00 21.71    B   N
ATOM  3695 CA  TYR B 217    -5.583  97.649  46.386  1.00 21.99    B   C
ATOM  3696 CB  TYR B 217    -5.307  96.167  46.658  1.00 22.18    B   C
ATOM  3697 CG  TYR B 217    -5.831  95.693  47.995  1.00 20.53    B   C
ATOM  3698 CD1 TYR B 217    -7.199  95.534  48.213  1.00 22.61    B   C
ATOM  3699 CE1 TYR B 217    -7.692  95.113  49.456  1.00 20.09    B   C
ATOM  3700 CD2 TYR B 217    -4.961  95.422  49.051  1.00 19.57    B   C
ATOM  3701 CE2 TYR B 217    -5.440  95.002  50.293  1.00 19.82    B   C
ATOM  3702 CZ  TYR B 217    -6.807  94.849  50.488  1.00 20.38    B   C
ATOM  3703 OH  TYR B 217    -7.288  94.422  51.709  1.00 19.08    B   O
ATOM  3704 C   TYR B 217    -5.056  98.473  47.558  1.00 22.00    B   C
ATOM  3705 O   TYR B 217    -5.832  98.992  48.362  1.00 21.85    B   O
ATOM  3706 N   LEU B 218    -3.734  98.591  47.654  1.00 19.08    B   N
ATOM  3707 CA  LEU B 218    -3.113  99.341  48.740  1.00 19.40    B   C
ATOM  3708 CB  LEU B 218    -1.585  99.279  48.615  1.00 17.82    B   C
ATOM  3709 CG  LEU B 218    -0.941  97.888  48.742  1.00 18.28    B   C
ATOM  3710 CD1 LEU B 218     0.541  97.968  48.389  1.00 15.96    B   C
ATOM  3711 CD2 LEU B 218    -1.128  97.353  50.155  1.00 16.26    B   C
ATOM  3712 C   LEU B 218    -3.582 100.798  48.791  1.00 21.94    B   C
ATOM  3713 O   LEU B 218    -3.841 101.335  49.866  1.00 18.51    B   O
ATOM  3714 N   GLN B 219    -3.691 101.433  47.629  1.00 22.92    B   N
ATOM  3715 CA  GLN B 219    -4.139 102.822  47.562  1.00 24.80    B   C
ATOM  3716 CB  GLN B 219    -4.004 103.353  46.129  1.00 26.04    B   C
ATOM  3717 CG  GLN B 219    -2.577 103.325  45.592  1.00 28.25    B   C
ATOM  3718 CD  GLN B 219    -2.470 103.820  44.156  1.00 28.07    B   C
ATOM  3719 OE1 GLN B 219    -3.166 103.334  43.262  1.00 25.98    B   O
ATOM  3720 NE2 GLN B 219    -1.588 104.790  43.932  1.00 30.48    B   N
ATOM  3721 C   GLN B 219    -5.596 102.914  48.005  1.00 24.27    B   C
ATOM  3722 O   GLN B 219    -5.995 103.859  48.683  1.00 25.16    B   O
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Figure 5NNN

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ATOM  3723  N   GLN B 220     -6.375 101.912  47.620  1.00 24.30      B   N
ATOM  3724  CA  GLN B 220     -7.792 101.838  47.943  1.00 28.00      B   C
ATOM  3725  CB  GLN B 220     -8.410 100.663  47.184  1.00 31.02      B   C
ATOM  3726  CG  GLN B 220     -9.920 100.674  47.077  1.00 39.36      B   C
ATOM  3727  CD  GLN B 220    -10.411 101.639  46.020  1.00 44.14      B   C
ATOM  3728  OE1 GLN B 220    -10.260 102.854  46.154  1.00 47.44      B   O
ATOM  3729  NE2 GLN B 220    -10.995 101.101  44.954  1.00 47.51      B   N
ATOM  3730  C   GLN B 220     -8.013 101.635  49.444  1.00 29.46      B   C
ATOM  3731  O   GLN B 220     -8.553 102.499  50.137  1.00 28.33      B   O
ATOM  3732  N   LYS B 221     -7.570 100.477  49.927  1.00 29.84      B   N
ATOM  3733  CA  LYS B 221     -7.720 100.075  51.321  1.00 28.05      B   C
ATOM  3734  CB  LYS B 221     -7.249  98.626  51.477  1.00 29.20      B   C
ATOM  3735  CG  LYS B 221     -8.124  97.761  52.381  1.00 33.06      B   C
ATOM  3736  CD  LYS B 221     -8.114  98.242  53.817  1.00 34.46      B   C
ATOM  3737  CE  LYS B 221     -8.796  97.239  54.738  1.00 34.63      B   C
ATOM  3738  NZ  LYS B 221     -8.003  95.993  54.896  1.00 31.31      B   N
ATOM  3739  C   LYS B 221     -7.012 100.953  52.345  1.00 27.08      B   C
ATOM  3740  O   LYS B 221     -7.556 101.230  53.416  1.00 27.24      B   O
ATOM  3741  N   TYR B 222     -5.804 101.399  52.029  1.00 25.82      B   N
ATOM  3742  CA  TYR B 222     -5.052 102.212  52.973  1.00 27.04      B   C
ATOM  3743  CB  TYR B 222     -3.658 101.616  53.147  1.00 22.44      B   C
ATOM  3744  CG  TYR B 222     -3.708 100.166  53.576  1.00 22.86      B   C
ATOM  3745  CD1 TYR B 222     -4.156  99.815  54.854  1.00 19.32      B   C
ATOM  3746  CE1 TYR B 222     -4.258  98.484  55.243  1.00 19.44      B   C
ATOM  3747  CD2 TYR B 222     -3.357  99.134  52.694  1.00 20.72      B   C
ATOM  3748  CE2 TYR B 222     -3.456  97.792  53.078  1.00 19.21      B   C
ATOM  3749  CZ  TYR B 222     -3.909  97.482  54.351  1.00 19.82      B   C
ATOM  3750  OH  TYR B 222     -4.027  96.167  54.725  1.00 19.05      B   O
ATOM  3751  C   TYR B 222     -4.968 103.667  52.539  1.00 29.48      B   C
ATOM  3752  O   TYR B 222     -4.096 104.405  52.986  1.00 31.72      B   O
ATOM  3753  N   ALA B 223     -5.900 104.089  51.696  1.00 32.87      B   N
ATOM  3754  CA  ALA B 223     -5.895 105.466  51.201  1.00 36.60      B   C
ATOM  3755  CB  ALA B 223     -6.672 106.421  52.148  1.00 37.41      B   C
ATOM  3756  C   ALA B 223     -4.442 105.909  51.088  1.00 38.06      B   C
ATOM  3757  O   ALA B 223     -4.060 106.977  51.560  1.00 38.78      B   O
ATOM  3758  N   LEU B 224     -3.627 105.088  50.441  1.00 38.57      B   N
ATOM  3759  CA  LEU B 224     -2.215 105.403  50.264  1.00 38.61      B   C
ATOM  3760  CB  LEU B 224     -1.402 104.097  50.136  1.00 39.37      B   C
ATOM  3761  CG  LEU B 224     -1.183 103.355  51.466  1.00 39.96      B   C
ATOM  3762  CD1 LEU B 224     -0.057 102.350  51.297  1.00 39.16      B   C
ATOM  3763  CD2 LEU B 224     -0.818 104.336  52.585  1.00 41.79      B   C
ATOM  3764  C   LEU B 224     -1.949 106.306  49.064  1.00 38.91      B   C
ATOM  3765  O   LEU B 224     -2.714 106.190  48.105  1.00 38.22      B   O
ATOM  3766  OXT LEU B 224     -0.969 107.085  49.068  1.00 39.30      B   O
ATOM  3767  CB  PRO B 232     11.684 106.007  48.754  1.00 35.25      B   C
ATOM  3768  CG  PRO B 232     11.385 107.285  47.963  1.00 36.48      B   C
ATOM  3769  C   PRO B 232     13.583 105.559  50.328  1.00 32.21      B   C
ATOM  3770  O   PRO B 232     14.407 105.139  49.517  1.00 33.63      B   O
ATOM  3771  N   PRO B 232     13.132 107.820  49.423  1.00 34.70      B   N
ATOM  3772  CD  PRO B 232     12.673 108.108  48.053  1.00 35.80      B   C
ATOM  3773  CA  PRO B 232     12.514 106.559  49.903  1.00 34.68      B   C
ATOM  3774  N   LYS B 233     13.566 105.183  51.602  1.00 30.94      B   N
ATOM  3775  CA  LYS B 233     14.542 104.237  52.126  1.00 27.68      B   C
ATOM  3776  CB  LYS B 233     14.693 104.412  53.637  1.00 30.73      B   C
ATOM  3777  CG  LYS B 233     15.074 105.817  54.076  1.00 37.18      B   C
ATOM  3778  CD  LYS B 233     15.073 105.930  55.594  1.00 41.29      B   C
ATOM  3779  CE  LYS B 233     15.358 107.357  56.045  1.00 46.10      B   C
ATOM  3780  NZ  LYS B 233     15.389 107.476  57.535  1.00 49.46      B   N
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Figure 5OOO

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ATOM  3781  C   LYS B 233     14.115 102.805  51.823  1.00 25.78    B   C
ATOM  3782  O   LYS B 233     12.984 102.404  52.108  1.00 21.74    B   O
ATOM  3783  N   VAL B 234     15.027 102.041  51.238  1.00 23.23    B   N
ATOM  3784  CA  VAL B 234     14.755 100.652  50.902  1.00 22.01    B   C
ATOM  3785  CB  VAL B 234     14.425 100.486  49.403  1.00 22.47    B   C
ATOM  3786  CG1 VAL B 234     14.095  99.034  49.105  1.00 23.89    B   C
ATOM  3787  CG2 VAL B 234     13.267 101.386  49.015  1.00 24.31    B   C
ATOM  3788  C   VAL B 234     15.997  99.825  51.204  1.00 21.91    B   C
ATOM  3789  O   VAL B 234     17.083 100.121  50.702  1.00 19.49    B   O
ATOM  3790  N   GLU B 235     15.850  98.805  52.041  1.00 19.26    B   N
ATOM  3791  CA  GLU B 235     16.987  97.956  52.343  1.00 19.57    B   C
ATOM  3792  CB  GLU B 235     17.407  98.085  53.812  1.00 22.19    B   C
ATOM  3793  CG  GLU B 235     16.367  97.736  54.849  1.00 27.30    B   C
ATOM  3794  CD  GLU B 235     16.893  97.954  56.266  1.00 31.20    B   C
ATOM  3795  OE1 GLU B 235     17.214  99.113  56.617  1.00 30.91    B   O
ATOM  3796  OE2 GLU B 235     16.992  96.967  57.027  1.00 31.05    B   O
ATOM  3797  C   GLU B 235     16.667  96.513  51.979  1.00 17.90    B   C
ATOM  3798  O   GLU B 235     15.514  96.071  52.067  1.00 17.20    B   O
ATOM  3799  N   PHE B 236     17.694  95.797  51.538  1.00 15.16    B   N
ATOM  3800  CA  PHE B 236     17.540  94.417  51.121  1.00 14.57    B   C
ATOM  3801  CB  PHE B 236     18.080  94.240  49.702  1.00 13.24    B   C
ATOM  3802  CG  PHE B 236     17.406  95.123  48.695  1.00 14.78    B   C
ATOM  3803  CD1 PHE B 236     17.807  96.448  48.529  1.00 13.54    B   C
ATOM  3804  CD2 PHE B 236     16.338  94.647  47.944  1.00 13.10    B   C
ATOM  3805  CE1 PHE B 236     17.148  97.281  47.625  1.00 15.52    B   C
ATOM  3806  CE2 PHE B 236     15.676  95.471  47.043  1.00 11.79    B   C
ATOM  3807  CZ  PHE B 236     16.083  96.792  46.884  1.00 13.41    B   C
ATOM  3808  C   PHE B 236     18.206  93.432  52.055  1.00 14.79    B   C
ATOM  3809  O   PHE B 236     19.298  93.668  52.566  1.00 14.15    B   O
ATOM  3810  N   HIS B 237     17.519  92.319  52.270  1.00 13.68    B   N
ATOM  3811  CA  HIS B 237     17.993  91.266  53.147  1.00 11.28    B   C
ATOM  3812  CB  HIS B 237     17.235  91.319  54.466  1.00 12.27    B   C
ATOM  3813  CG  HIS B 237     17.437  92.597  55.219  1.00 14.02    B   C
ATOM  3814  CD2 HIS B 237     16.779  93.778  55.159  1.00 14.88    B   C
ATOM  3815  ND1 HIS B 237     18.460  92.771  56.126  1.00 14.41    B   N
ATOM  3816  CE1 HIS B 237     18.423  94.006  56.593  1.00 18.35    B   C
ATOM  3817  NE2 HIS B 237     17.413  94.638  56.023  1.00 14.90    B   N
ATOM  3818  C   HIS B 237     17.705  89.961  52.437  1.00 13.01    B   C
ATOM  3819  O   HIS B 237     16.725  89.860  51.702  1.00 12.07    B   O
ATOM  3820  N   ALA B 238     18.554  88.967  52.665  1.00 12.63    B   N
ATOM  3821  CA  ALA B 238     18.387  87.671  52.022  1.00 11.54    B   C
ATOM  3822  CB  ALA B 238     19.018  87.700  50.639  1.00  9.85    B   C
ATOM  3823  C   ALA B 238     19.010  86.554  52.836  1.00 14.48    B   C
ATOM  3824  O   ALA B 238     19.998  86.765  53.533  1.00 14.69    B   O
ATOM  3825  N   SER B 239     18.424  85.364  52.741  1.00 14.68    B   N
ATOM  3826  CA  SER B 239     18.948  84.202  53.447  1.00 14.80    B   C
ATOM  3827  CB  SER B 239     17.862  83.141  53.608  1.00 13.43    B   C
ATOM  3828  OG  SER B 239     17.340  82.758  52.355  1.00 13.26    B   O
ATOM  3829  C   SER B 239     20.104  83.656  52.614  1.00 14.91    B   C
ATOM  3830  O   SER B 239     20.945  82.902  53.107  1.00 12.99    B   O
ATOM  3831  N   GLY B 240     20.134  84.050  51.344  1.00 14.12    B   N
ATOM  3832  CA  GLY B 240     21.197  83.631  50.455  1.00 15.59    B   C
ATOM  3833  C   GLY B 240     22.217  84.752  50.346  1.00 16.66    B   C
ATOM  3834  O   GLY B 240     22.520  85.416  51.334  1.00 16.99    B   O
ATOM  3835  N   ASP B 241     22.732  84.985  49.145  1.00 15.94    B   N
ATOM  3836  CA  ASP B 241     23.722  86.036  48.947  1.00 17.18    B   C
ATOM  3837  CB  ASP B 241     24.487  85.795  47.649  1.00 18.32    B   C
ATOM  3838  CG  ASP B 241     25.703  86.673  47.527  1.00 21.73    B   C
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Figure 5PPP

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ATOM  3839 OD1 ASP B 241     25.702  87.771  48.126  1.00 22.80    B   O
ATOM  3840 OD2 ASP B 241     26.653  86.277  46.824  1.00 23.86    B   O
ATOM  3841 C   ASP B 241     23.070  87.416  48.899  1.00 15.91    B   C
ATOM  3842 O   ASP B 241     22.566  87.838  47.855  1.00 18.69    B   O
ATOM  3843 N   VAL B 242     23.091  88.125  50.022  1.00 15.82    B   N
ATOM  3844 CA  VAL B 242     22.480  89.447  50.079  1.00 15.47    B   C
ATOM  3845 CB  VAL B 242     22.373  89.961  51.538  1.00 14.55    B   C
ATOM  3846 CG1 VAL B 242     23.753  90.329  52.079  1.00 14.67    B   C
ATOM  3847 CG2 VAL B 242     21.405  91.147  51.599  1.00 13.95    B   C
ATOM  3848 C   VAL B 242     23.230  90.480  49.242  1.00 16.20    B   C
ATOM  3849 O   VAL B 242     22.624  91.396  48.693  1.00 16.97    B   O
ATOM  3850 N   ILE B 243     24.546  90.347  49.145  1.00 15.87    B   N
ATOM  3851 CA  ILE B 243     25.307  91.303  48.351  1.00 15.88    B   C
ATOM  3852 CB  ILE B 243     26.833  91.076  48.512  1.00 17.32    B   C
ATOM  3853 CG2 ILE B 243     27.606  91.924  47.510  1.00 17.19    B   C
ATOM  3854 CG1 ILE B 243     27.249  91.447  49.940  1.00 19.37    B   C
ATOM  3855 CD1 ILE B 243     28.685  91.096  50.286  1.00 19.42    B   C
ATOM  3856 C   ILE B 243     24.882  91.191  46.889  1.00 14.23    B   C
ATOM  3857 O   ILE B 243     24.745  92.200  46.201  1.00 14.19    B   O
ATOM  3858 N   TRP B 244     24.651  89.967  46.421  1.00 14.60    B   N
ATOM  3859 CA  TRP B 244     24.207  89.756  45.046  1.00 14.98    B   C
ATOM  3860 CB  TRP B 244     24.078  88.264  44.729  1.00 15.60    B   C
ATOM  3861 CG  TRP B 244     23.575  87.999  43.329  1.00 16.65    B   C
ATOM  3862 CD2 TRP B 244     22.210  87.806  42.930  1.00 19.35    B   C
ATOM  3863 CE2 TRP B 244     22.206  87.617  41.527  1.00 18.45    B   C
ATOM  3864 CE3 TRP B 244     20.989  87.775  43.622  1.00 18.90    B   C
ATOM  3865 CD1 TRP B 244     24.321  87.924  42.184  1.00 18.57    B   C
ATOM  3866 NE1 TRP B 244     23.506  87.694  41.097  1.00 17.92    B   N
ATOM  3867 CZ2 TRP B 244     21.029  87.398  40.803  1.00 17.47    B   C
ATOM  3868 CZ3 TRP B 244     19.818  87.558  42.902  1.00 18.34    B   C
ATOM  3869 CH2 TRP B 244     19.847  87.371  41.504  1.00 17.51    B   C
ATOM  3870 C   TRP B 244     22.845  90.409  44.850  1.00 16.58    B   C
ATOM  3871 O   TRP B 244     22.616  91.102  43.859  1.00 17.56    B   O
ATOM  3872 N   LEU B 245     21.937  90.180  45.796  1.00 15.30    B   N
ATOM  3873 CA  LEU B 245     20.599  90.749  45.707  1.00 15.38    B   C
ATOM  3874 CB  LEU B 245     19.746  90.306  46.900  1.00 14.42    B   C
ATOM  3875 CG  LEU B 245     18.287  90.782  46.894  1.00 12.51    B   C
ATOM  3876 CD1 LEU B 245     17.536  90.163  45.723  1.00 15.01    B   C
ATOM  3877 CD2 LEU B 245     17.618  90.397  48.215  1.00 15.46    B   C
ATOM  3878 C   LEU B 245     20.648  92.270  45.660  1.00 15.93    B   C
ATOM  3879 O   LEU B 245     19.895  92.901  44.916  1.00 11.84    B   O
ATOM  3880 N   GLU B 246     21.534  92.865  46.454  1.00 16.60    B   N
ATOM  3881 CA  GLU B 246     21.636  94.317  46.480  1.00 17.29    B   C
ATOM  3882 CB  GLU B 246     22.496  94.782  47.658  1.00 18.17    B   C
ATOM  3883 CG  GLU B 246     21.896  94.455  49.020  1.00 19.87    B   C
ATOM  3884 CD  GLU B 246     22.776  94.908  50.176  1.00 21.82    B   C
ATOM  3885 OE1 GLU B 246     24.001  94.687  50.101  1.00 23.59    B   O
ATOM  3886 OE2 GLU B 246     22.244  95.471  51.161  1.00 18.84    B   O
ATOM  3887 C   GLU B 246     22.213  94.819  45.171  1.00 19.10    B   C
ATOM  3888 O   GLU B 246     21.866  95.905  44.711  1.00 18.10    B   O
ATOM  3889 N   ARG B 247     23.082  94.016  44.564  1.00 20.90    B   N
ATOM  3890 CA  ARG B 247     23.694  94.384  43.296  1.00 21.36    B   C
ATOM  3891 CB  ARG B 247     24.819  93.407  42.945  1.00 23.57    B   C
ATOM  3892 CG  ARG B 247     25.698  93.843  41.780  1.00 28.81    B   C
ATOM  3893 CD  ARG B 247     26.796  92.813  41.516  1.00 31.64    B   C
ATOM  3894 NE  ARG B 247     27.648  92.622  42.688  1.00 33.01    B   N
ATOM  3895 CZ  ARG B 247     27.953  91.437  43.214  1.00 34.15    B   C
ATOM  3896 NH1 ARG B 247     27.475  90.319  42.678  1.00 32.31    B   N
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Figure 5QQQ

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ATOM  3897 NH2 ARG B 247     28.742  91.372  44.281  1.00 32.59      B   N
ATOM  3898 C   ARG B 247     22.612  94.369  42.218  1.00 21.28      B   C
ATOM  3899 O   ARG B 247     22.613  95.212  41.319  1.00 18.68      B   O
ATOM  3900 N   GLN B 248     21.689  93.411  42.316  1.00 19.88      B   N
ATOM  3901 CA  GLN B 248     20.587  93.310  41.359  1.00 18.33      B   C
ATOM  3902 CB  GLN B 248     19.778  92.027  41.586  1.00 16.87      B   C
ATOM  3903 CG  GLN B 248     20.458  90.749  41.119  1.00 17.30      B   C
ATOM  3904 CD  GLN B 248     20.794  90.768  39.631  1.00 21.87      B   C
ATOM  3905 OE1 GLN B 248     19.946  91.077  38.790  1.00 23.30      B   O
ATOM  3906 NE2 GLN B 248     22.032  90.423  39.304  1.00 24.03      B   N
ATOM  3907 C   GLN B 248     19.670  94.518  41.528  1.00 17.34      B   C
ATOM  3908 O   GLN B 248     19.166  95.071  40.550  1.00 16.87      B   O
ATOM  3909 N   ALA B 249     19.451  94.917  42.777  1.00 15.06      B   N
ATOM  3910 CA  ALA B 249     18.598  96.069  43.059  1.00 17.68      B   C
ATOM  3911 CB  ALA B 249     18.435  96.240  44.557  1.00 14.89      B   C
ATOM  3912 C   ALA B 249     19.210  97.332  42.449  1.00 16.19      B   C
ATOM  3913 O   ALA B 249     18.509  98.166  41.878  1.00 15.71      B   O
ATOM  3914 N   LYS B 250     20.523  97.466  42.578  1.00 15.67      B   N
ATOM  3915 CA  LYS B 250     21.221  98.625  42.039  1.00 16.75      B   C
ATOM  3916 CB  LYS B 250     22.686  98.599  42.493  1.00 20.71      B   C
ATOM  3917 CG  LYS B 250     23.555  99.725  41.952  1.00 24.70      B   C
ATOM  3918 CD  LYS B 250     23.089 101.093  42.425  1.00 29.48      B   C
ATOM  3919 CE  LYS B 250     24.028 102.180  41.914  1.00 34.06      B   C
ATOM  3920 NZ  LYS B 250     23.548 103.549  42.249  1.00 35.09      B   N
ATOM  3921 C   LYS B 250     21.137  98.633  40.514  1.00 16.02      B   C
ATOM  3922 O   LYS B 250     20.910  99.672  39.899  1.00 16.61      B   O
ATOM  3923 N   GLU B 251     21.300  97.464  39.907  1.00 16.92      B   N
ATOM  3924 CA  GLU B 251     21.256  97.366  38.457  1.00 16.87      B   C
ATOM  3925 CB  GLU B 251     21.789  96.009  38.000  1.00 17.15      B   C
ATOM  3926 CG  GLU B 251     21.913  95.902  36.492  1.00 19.76      B   C
ATOM  3927 CD  GLU B 251     22.195  94.495  36.030  1.00 21.03      B   C
ATOM  3928 OE1 GLU B 251     22.812  93.728  36.796  1.00 21.54      B   O
ATOM  3929 OE2 GLU B 251     21.813  94.159  34.891  1.00 23.50      B   O
ATOM  3930 C   GLU B 251     19.864  97.561  37.868  1.00 18.30      B   C
ATOM  3931 O   GLU B 251     19.696  98.297  36.895  1.00 18.23      B   O
ATOM  3932 N   TRP B 252     18.865  96.918  38.464  1.00 17.41      B   N
ATOM  3933 CA  TRP B 252     17.509  96.997  37.939  1.00 17.31      B   C
ATOM  3934 CB  TRP B 252     16.868  95.610  37.973  1.00 16.21      B   C
ATOM  3935 CG  TRP B 252     17.639  94.610  37.197  1.00 16.40      B   C
ATOM  3936 CD2 TRP B 252     17.650  94.459  35.775  1.00 17.43      B   C
ATOM  3937 CE2 TRP B 252     18.546  93.412  35.475  1.00 17.08      B   C
ATOM  3938 CE3 TRP B 252     16.988  95.107  34.723  1.00 20.12      B   C
ATOM  3939 CD1 TRP B 252     18.505  93.677  37.690  1.00 18.25      B   C
ATOM  3940 NE1 TRP B 252     19.053  92.954  36.662  1.00 17.57      B   N
ATOM  3941 CZ2 TRP B 252     18.799  92.996  34.167  1.00 16.27      B   C
ATOM  3942 CZ3 TRP B 252     17.239  94.691  33.416  1.00 18.36      B   C
ATOM  3943 CH2 TRP B 252     18.137  93.646  33.153  1.00 18.85      B   C
ATOM  3944 C   TRP B 252     16.555  98.000  38.565  1.00 20.68      B   C
ATOM  3945 O   TRP B 252     15.631  98.468  37.896  1.00 23.26      B   O
ATOM  3946 N   LEU B 253     16.762  98.333  39.833  1.00 20.19      B   N
ATOM  3947 CA  LEU B 253     15.878  99.279  40.508  1.00 22.15      B   C
ATOM  3948 CB  LEU B 253     15.392  98.680  41.832  1.00 19.99      B   C
ATOM  3949 CG  LEU B 253     14.796  97.269  41.748  1.00 20.08      B   C
ATOM  3950 CD1 LEU B 253     14.520  96.731  43.149  1.00 15.94      B   C
ATOM  3951 CD2 LEU B 253     13.521  97.299  40.918  1.00 20.16      B   C
ATOM  3952 C   LEU B 253     16.588 100.602  40.766  1.00 25.98      B   C
ATOM  3953 O   LEU B 253     15.971 101.573  41.213  1.00 28.88      B   O
ATOM  3954 N   LYS B 254     17.887 100.631  40.478  1.00 28.33      B   N
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Figure 5RRR

```
ATOM  3955 CA  LYS B 254     18.713 101.822  40.684  1.00 32.00      B   C
ATOM  3956 CB  LYS B 254     18.210 102.985  39.818  1.00 33.97      B   C
ATOM  3957 CG  LYS B 254     17.844 102.597  38.388  1.00 37.77      B   C
ATOM  3958 CD  LYS B 254     18.983 101.890  37.661  1.00 38.80      B   C
ATOM  3959 CE  LYS B 254     18.544 101.453  36.265  1.00 41.63      B   C
ATOM  3960 NZ  LYS B 254     19.608 100.705  35.535  1.00 41.49      B   N
ATOM  3961 C   LYS B 254     18.677 102.214  42.162  1.00 32.29      B   C
ATOM  3962 O   LYS B 254     18.716 103.399  42.511  1.00 32.23      B   O
ATOM  3963 N   LEU B 255     18.603 101.201  43.022  1.00 31.24      B   N
ATOM  3964 CA  LEU B 255     18.560 101.397  44.469  1.00 34.52      B   C
ATOM  3965 CB  LEU B 255     17.250 100.844  45.039  1.00 34.04      B   C
ATOM  3966 CG  LEU B 255     15.917 101.437  44.584  1.00 36.59      B   C
ATOM  3967 CD1 LEU B 255     14.795 100.596  45.162  1.00 35.66      B   C
ATOM  3968 CD2 LEU B 255     15.791 102.888  45.036  1.00 36.85      B   C
ATOM  3969 C   LEU B 255     19.727 100.667  45.132  1.00 35.40      B   C
ATOM  3970 O   LEU B 255     20.326  99.794  44.473  1.00 34.56      B   O
ATOM  3971 OXT LEU B 255     20.014 100.959  46.310  1.00 38.02      B   O
ATOM  3972 N   GLD G 301     22.488  67.641  43.303  1.00  8.65      G   N
ATOM  3973 CA  GLD G 301     22.952  68.704  42.405  1.00 12.93      G   C
ATOM  3974 CB  GLD G 301     21.889  69.041  41.338  1.00 11.63      G   C
ATOM  3975 CG  GLD G 301     20.594  69.573  41.934  1.00 12.92      G   C
ATOM  3976 CD  GLD G 301     20.824  70.895  42.710  1.00 11.91      G   C
ATOM  3977 OE1 GLD G 301     21.256  71.889  42.077  1.00  9.76      G   O
ATOM  3978 OE2 GLD G 301     20.616  70.917  43.937  1.00 14.58      G   O
ATOM  3979 C   GLD G 301     24.267  68.360  41.735  1.00 11.46      G   C
ATOM  3980 O   GLD G 301     24.630  67.169  41.697  1.00 11.93      G   O
ATOM  3981 O1  GLD G 301     24.920  69.308  41.262  1.00 13.36      G   O
ATOM  3982 N   GLD H 302      8.053  83.746  43.978  1.00 11.84      H   N
ATOM  3983 CA  GLD H 302      7.425  82.601  43.310  1.00 14.35      H   C
ATOM  3984 CB  GLD H 302      8.287  82.089  42.143  1.00 12.93      H   C
ATOM  3985 CG  GLD H 302      9.638  81.579  42.619  1.00 15.67      H   C
ATOM  3986 CD  GLD H 302      9.448  80.386  43.597  1.00 14.81      H   C
ATOM  3987 OE1 GLD H 302      8.878  79.354  43.166  1.00 15.24      H   O
ATOM  3988 OE2 GLD H 302      9.825  80.506  44.780  1.00 14.34      H   O
ATOM  3989 C   GLD H 302      6.027  82.912  42.821  1.00 13.03      H   C
ATOM  3990 O   GLD H 302      5.676  84.098  42.749  1.00 11.51      H   O
ATOM  3991 O1  GLD H 302      5.308  81.938  42.528  1.00 15.43      H   O
ATOM  4058 OH2 TIP S   1     26.694  70.185  39.535  1.00 10.43      S   O
ATOM  4059 OH2 TIP S   2     26.903  61.775  37.433  1.00 10.86      S   O
ATOM  4060 OH2 TIP S   3     35.118  64.928  45.661  1.00  9.77      S   O
ATOM  4061 OH2 TIP S   4      3.740  88.714  42.243  1.00 12.17      S   O
ATOM  4062 OH2 TIP S   5     -3.817  87.331  48.367  1.00 15.62      S   O
ATOM  4063 OH2 TIP S   6     16.515  80.411  54.861  1.00 15.64      S   O
ATOM  4064 OH2 TIP S   7     26.620  62.820  41.255  1.00 10.32      S   O
ATOM  4065 OH2 TIP S   8      3.173  81.112  41.277  1.00 12.87      S   O
ATOM  4066 OH2 TIP S   9     -5.009  77.145  39.859  1.00 14.54      S   O
ATOM  4067 OH2 TIP S  10     17.072  78.274  43.100  1.00 15.49      S   O
ATOM  4068 OH2 TIP S  11     11.094  82.014  54.953  1.00 13.66      S   O
ATOM  4069 OH2 TIP S  12     23.114  78.487  54.347  1.00 14.98      S   O
ATOM  4070 OH2 TIP S  13     20.046  86.513  47.218  1.00 13.55      S   O
ATOM  4071 OH2 TIP S  14      2.655  89.017  38.291  1.00 15.07      S   O
ATOM  4072 OH2 TIP S  15      9.228  70.350  55.121  1.00 12.46      S   O
ATOM  4073 OH2 TIP S  16     16.739  84.862  44.381  1.00 12.76      S   O
ATOM  4074 OH2 TIP S  17     25.567  61.078  39.581  1.00 14.41      S   O
ATOM  4075 OH2 TIP S  18     37.252  56.626  40.690  1.00 14.19      S   O
ATOM  4076 OH2 TIP S  19     18.275  89.911  32.191  1.00 17.34      S   O
ATOM  4077 OH2 TIP S  20     34.008  72.385  38.024  1.00 14.04      S   O
ATOM  4078 OH2 TIP S  21     -1.688  79.172  55.257  1.00 19.38      S   O
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Figure 5SSS

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ATOM  4079  OH2 TIP S  22      22.366  80.667  29.821  1.00 24.75      S   O
ATOM  4080  OH2 TIP S  23      12.380  75.091  59.029  1.00 20.05      S   O
ATOM  4081  OH2 TIP S  24      22.730  75.591  37.990  1.00 18.05      S   O
ATOM  4082  OH2 TIP S  25      -4.035  89.431  50.414  1.00 17.74      S   O
ATOM  4083  OH2 TIP S  26       4.573  89.940  39.949  1.00 14.11      S   O
ATOM  4084  OH2 TIP S  27      -1.906  87.737  40.180  1.00 17.43      S   O
ATOM  4085  OH2 TIP S  28      10.589  69.698  44.737  1.00 21.71      S   O
ATOM  4086  OH2 TIP S  29      25.201  95.439  52.148  1.00 16.83      S   O
ATOM  4087  OH2 TIP S  30      -8.367  85.700  23.246  1.00 15.98      S   O
ATOM  4088  OH2 TIP S  31      35.982  63.130  47.769  1.00 15.06      S   O
ATOM  4089  OH2 TIP S  32      21.296  70.481  54.804  1.00 19.30      S   O
ATOM  4090  OH2 TIP S  33      20.570  73.504  39.900  1.00 18.13      S   O
ATOM  4091  OH2 TIP S  34      27.666  49.772  40.587  1.00 14.52      S   O
ATOM  4092  OH2 TIP S  35       9.700  74.285  55.955  1.00 16.17      S   O
ATOM  4093  OH2 TIP S  36      12.186  64.800  48.529  1.00 17.60      S   O
ATOM  4094  OH2 TIP S  37      13.322  82.831  56.421  1.00 13.15      S   O
ATOM  4095  OH2 TIP S  38      34.693  38.751  49.392  1.00 20.67      S   O
ATOM  4096  OH2 TIP S  39      -5.001  91.649  54.454  1.00 20.34      S   O
ATOM  4097  OH2 TIP S  40      15.761  67.824  58.496  1.00 21.39      S   O
ATOM  4098  OH2 TIP S  41      11.148  84.424  43.877  1.00 12.67      S   O
ATOM  4099  OH2 TIP S  42      37.642  61.003  46.856  1.00 17.93      S   O
ATOM  4100  OH2 TIP S  43      -4.373  79.173  41.785  1.00 16.71      S   O
ATOM  4101  OH2 TIP S  44      43.723  52.077  51.584  1.00 18.94      S   O
ATOM  4102  OH2 TIP S  45      20.137  97.010  51.207  1.00 22.61      S   O
ATOM  4103  OH2 TIP S  46      -4.186  94.391  33.354  1.00 24.48      S   O
ATOM  4104  OH2 TIP S  47      10.434  59.744  34.860  1.00 20.09      S   O
ATOM  4105  OH2 TIP S  48      11.296  69.306  47.243  1.00 20.43      S   O
ATOM  4106  OH2 TIP S  49      13.514  84.678  43.033  1.00 17.25      S   O
ATOM  4107  OH2 TIP S  50      27.738  70.677  61.698  1.00 22.46      S   O
ATOM  4108  OH2 TIP S  51      16.289  72.356  55.129  1.00 13.74      S   O
ATOM  4109  OH2 TIP S  52      -4.477  95.904  37.489  1.00 27.31      S   O
ATOM  4110  OH2 TIP S  53      34.164  74.207  35.803  1.00 16.19      S   O
ATOM  4111  OH2 TIP S  54      13.181  73.070  43.734  1.00 17.17      S   O
ATOM  4112  OH2 TIP S  55      -3.958  90.260  57.512  1.00 25.11      S   O
ATOM  4113  OH2 TIP S  56      30.703  42.485  54.038  1.00 21.11      S   O
ATOM  4114  OH2 TIP S  57      30.922  56.349  27.885  1.00 20.13      S   O
ATOM  4115  OH2 TIP S  58      14.662  74.601  55.720  1.00 22.72      S   O
ATOM  4116  OH2 TIP S  59      38.507  59.138  50.812  1.00 19.14      S   O
ATOM  4117  OH2 TIP S  60      42.816  67.475  28.609  1.00 20.79      S   O
ATOM  4118  OH2 TIP S  61      -6.400  95.465  43.206  1.00 18.25      S   O
ATOM  4119  OH2 TIP S  62       6.561 102.864  47.606  1.00 21.89      S   O
ATOM  4120  OH2 TIP S  63      35.560  76.427  29.271  1.00 20.86      S   O
ATOM  4121  OH2 TIP S  64       5.810  69.019  32.123  1.00 25.31      S   O
ATOM  4122  OH2 TIP S  65      30.127  54.457  33.804  1.00 22.20      S   O
ATOM  4123  OH2 TIP S  66      14.517  98.509  59.915  1.00 20.97      S   O
ATOM  4124  OH2 TIP S  67      20.921  81.728  55.488  1.00 15.12      S   O
ATOM  4125  OH2 TIP S  68      18.125  78.127  55.061  1.00 22.38      S   O
ATOM  4126  OH2 TIP S  69       4.578 106.224  53.414  1.00 23.88      S   O
ATOM  4127  OH2 TIP S  70     -13.259  95.151  42.403  1.00 22.02      S   O
ATOM  4128  OH2 TIP S  71      19.506  66.848  43.948  1.00 14.64      S   O
ATOM  4129  OH2 TIP S  72      20.492  58.168  29.357  1.00 24.23      S   O
ATOM  4130  OH2 TIP S  73      14.362  66.682  45.311  1.00 21.95      S   O
ATOM  4131  OH2 TIP S  74      37.948  64.500  49.199  1.00 22.89      S   O
ATOM  4132  OH2 TIP S  75      22.382  83.107  46.881  1.00 21.36      S   O
ATOM  4133  OH2 TIP S  76       2.257  71.707  33.743  1.00 22.26      S   O
ATOM  4134  OH2 TIP S  77      28.562  50.607  60.811  1.00 23.59      S   O
ATOM  4135  OH2 TIP S  78      12.908  55.269  54.605  1.00 22.04      S   O
ATOM  4136  OH2 TIP S  79      23.712  82.581  52.850  1.00 18.46      S   O
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Figure 5TTT

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ATOM  4137  OH2 TIP S  80      6.000  64.702  50.376  1.00 22.24      S   O
ATOM  4138  OH2 TIP S  81     31.597  63.665  38.013  1.00 16.06      S   O
ATOM  4139  OH2 TIP S  82      3.204 101.393  39.851  1.00 18.09      S   O
ATOM  4140  OH2 TIP S  83     -3.695  88.746  62.013  1.00 24.84      S   O
ATOM  4141  OH2 TIP S  84     17.546  65.110  21.326  1.00 19.55      S   O
ATOM  4142  OH2 TIP S  85     26.824  59.347  62.759  1.00 26.30      S   O
ATOM  4143  OH2 TIP S  86     29.013  78.700  36.194  1.00 29.19      S   O
ATOM  4144  OH2 TIP S  87    -21.912  84.760  37.477  1.00 26.29      S   O
ATOM  4145  OH2 TIP S  88     37.659  49.564  54.905  1.00 21.54      S   O
ATOM  4146  OH2 TIP S  89     15.623  89.654  61.494  1.00 20.60      S   O
ATOM  4147  OH2 TIP S  90     46.913  73.636  27.864  1.00 24.09      S   O
ATOM  4148  OH2 TIP S  91     31.635  68.716  13.795  1.00 26.68      S   O
ATOM  4149  OH2 TIP S  92      8.998  77.444  41.106  1.00 21.52      S   O
ATOM  4150  OH2 TIP S  93     19.563  69.848  56.803  1.00 23.78      S   O
ATOM  4151  OH2 TIP S  94     21.054  77.796  57.903  1.00 20.91      S   O
ATOM  4152  OH2 TIP S  95     39.029  70.195  42.752  1.00 19.43      S   O
ATOM  4153  OH2 TIP S  96     16.357  59.879  28.472  1.00 34.72      S   O
ATOM  4154  OH2 TIP S  97      6.277  85.600  21.656  1.00 18.30      S   O
ATOM  4155  OH2 TIP S  98     24.381  79.010  25.797  1.00 24.45      S   O
ATOM  4156  OH2 TIP S  99     -0.330  73.515  46.326  1.00 21.44      S   O
ATOM  4157  OH2 TIP S 100     19.996  63.469  21.479  1.00 20.07      S   O
ATOM  4158  OH2 TIP S 101      8.484  64.804  37.057  1.00 21.03      S   O
ATOM  4159  OH2 TIP S 102     18.063  76.067  36.689  1.00 20.99      S   O
ATOM  4160  OH2 TIP S 103     13.804  68.104  43.044  1.00 25.16      S   O
ATOM  4161  OH2 TIP S 104     10.019  70.355  50.629  1.00 23.39      S   O
ATOM  4162  OH2 TIP S 105     36.764  63.450  55.390  1.00 19.23      S   O
ATOM  4163  OH2 TIP S 106     -3.017  81.106  52.043  1.00 29.08      S   O
ATOM  4164  OH2 TIP S 107     33.894  73.874  51.602  1.00 22.56      S   O
ATOM  4165  OH2 TIP S 108    -10.562  79.620  30.884  1.00 25.06      S   O
ATOM  4166  OH2 TIP S 109     -3.241  87.887  16.187  1.00 22.20      S   O
ATOM  4167  OH2 TIP S 110     36.320  79.997  40.961  1.00 30.47      S   O
ATOM  4168  OH2 TIP S 111     12.536  71.003  57.233  1.00 20.62      S   O
ATOM  4169  OH2 TIP S 112     -0.943  95.950  34.554  1.00 25.68      S   O
ATOM  4170  OH2 TIP S 113     14.938  45.779  46.539  1.00 32.69      S   O
ATOM  4171  OH2 TIP S 114     44.541  72.750  24.779  1.00 28.57      S   O
ATOM  4172  OH2 TIP S 115     16.028  56.338  61.884  1.00 27.69      S   O
ATOM  4173  OH2 TIP S 116     25.959  84.862  44.510  1.00 22.27      S   O
ATOM  4174  OH2 TIP S 117     11.898  70.641  40.303  1.00 29.38      S   O
ATOM  4175  OH2 TIP S 118     20.005  82.352  45.778  1.00 23.69      S   O
ATOM  4176  OH2 TIP S 119     24.653  82.113  42.509  1.00 26.73      S   O
ATOM  4177  OH2 TIP S 120     39.045  70.244  55.129  1.00 26.86      S   O
ATOM  4178  OH2 TIP S 121    -14.861  94.263  30.815  1.00 25.70      S   O
ATOM  4179  OH2 TIP S 122     28.805  79.348  55.384  1.00 24.42      S   O
ATOM  4180  OH2 TIP S 123     34.409  78.819  35.704  1.00 22.51      S   O
ATOM  4181  OH2 TIP S 124     25.708  95.887  48.431  1.00 22.52      S   O
ATOM  4182  OH2 TIP S 125     20.200  81.715  43.235  1.00 28.28      S   O
ATOM  4183  OH2 TIP S 126      8.358  89.545  27.306  1.00 25.44      S   O
ATOM  4184  OH2 TIP S 127     28.451  42.142  55.370  1.00 32.71      S   O
ATOM  4185  OH2 TIP S 128     -1.140  72.535  35.377  1.00 25.03      S   O
ATOM  4186  OH2 TIP S 129     42.723  73.261  29.197  1.00 26.01      S   O
ATOM  4187  OH2 TIP S 130      0.475 106.754  43.565  1.00 35.60      S   O
ATOM  4188  OH2 TIP S 131     -8.799  81.517  47.238  1.00 30.82      S   O
ATOM  4189  OH2 TIP S 132     18.817  63.647  62.682  1.00 23.39      S   O
ATOM  4190  OH2 TIP S 133    -14.788  83.367  33.703  1.00 22.25      S   O
ATOM  4191  OH2 TIP S 134     28.486  47.289  40.587  1.00 26.04      S   O
ATOM  4192  OH2 TIP S 135     13.709  66.288  58.292  1.00 31.84      S   O
ATOM  4193  OH2 TIP S 136      4.869  72.011  43.934  1.00 21.85      S   O
ATOM  4194  OH2 TIP S 137    -19.103  77.442  35.205  1.00 29.80      S   O
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Figure 5UUU

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ATOM  4195  OH2 TIP S 138     20.407  79.490  35.831  1.00 35.16      S   O
ATOM  4196  OH2 TIP S 139     10.860  84.010  22.443  1.00 27.02      S   O
ATOM  4197  OH2 TIP S 140      0.151 101.506  60.922  1.00 25.88      S   O
ATOM  4198  OH2 TIP S 141     31.584  47.279  41.254  1.00 23.80      S   O
ATOM  4199  OH2 TIP S 142     38.066  70.701  25.990  1.00 19.24      S   O
ATOM  4200  OH2 TIP S 143     44.977  72.631  31.204  1.00 23.78      S   O
ATOM  4201  OH2 TIP S 144     10.719  65.231  40.054  1.00 26.38      S   O
ATOM  4202  OH2 TIP S 145      7.475  91.297  29.034  1.00 27.02      S   O
ATOM  4203  OH2 TIP S 146     37.874  61.748  52.268  1.00 29.73      S   O
ATOM  4204  OH2 TIP S 147     -5.574  93.894  53.509  1.00 23.66      S   O
ATOM  4205  OH2 TIP S 148     17.820  78.905  36.654  1.00 28.79      S   O
ATOM  4206  OH2 TIP S 149     29.549  83.050  48.881  1.00 26.52      S   O
ATOM  4207  OH2 TIP S 150    -10.366 100.932  54.067  1.00 20.68      S   O
ATOM  4208  OH2 TIP S 151     30.504  64.646  60.794  1.00 28.37      S   O
ATOM  4209  OH2 TIP S 152     49.012  70.756  24.772  1.00 31.55      S   O
ATOM  4210  OH2 TIP S 153     30.846  45.257  57.188  1.00 31.72      S   O
ATOM  4211  OH2 TIP S 154     43.180  59.055  25.923  1.00 26.29      S   O
ATOM  4212  OH2 TIP S 155     22.523  66.585  65.647  1.00 32.96      S   O
ATOM  4213  OH2 TIP S 156      2.253 106.632  56.997  1.00 37.06      S   O
ATOM  4214  OH2 TIP S 157     21.987  90.927  36.214  1.00 24.25      S   O
ATOM  4215  OH2 TIP S 158     24.995  45.779  50.248  1.00 28.19      S   O
ATOM  4216  OH2 TIP S 159     24.701  87.274  52.417  1.00 25.41      S   O
ATOM  4217  OH2 TIP S 160     19.481  54.793  61.669  1.00 24.28      S   O
ATOM  4218  OH2 TIP S 161      5.052  66.267  52.559  1.00 20.50      S   O
ATOM  4219  OH2 TIP S 162     24.083  47.425  48.238  1.00 32.20      S   O
ATOM  4220  OH2 TIP S 163     50.567  67.161  31.028  1.00 21.83      S   O
ATOM  4221  OH2 TIP S 164     15.358  64.805  23.213  1.00 24.49      S   O
ATOM  4222  OH2 TIP S 165     -1.913  91.256  42.961  1.00 21.23      S   O
ATOM  4223  OH2 TIP S 166     32.576  60.552  40.991  1.00 24.61      S   O
ATOM  4224  OH2 TIP S 167      5.829  70.768  57.525  1.00 22.41      S   O
ATOM  4225  OH2 TIP S 168      6.357  83.074  62.946  1.00 20.77      S   O
ATOM  4226  OH2 TIP S 169     28.962  85.053  47.200  1.00 36.42      S   O
ATOM  4227  OH2 TIP S 170     22.828  55.785  37.965  1.00 34.04      S   O
ATOM  4228  OH2 TIP S 171      9.903 109.166  51.388  1.00 29.79      S   O
ATOM  4229  OH2 TIP S 172      6.629  71.093  33.592  1.00 24.39      S   O
ATOM  4230  OH2 TIP S 173     24.428  80.747  55.009  1.00 17.22      S   O
ATOM  4231  OH2 TIP S 174     11.049  67.896  25.243  1.00 28.73      S   O
ATOM  4232  OH2 TIP S 175     26.525  84.672  50.346  1.00 22.59      S   O
ATOM  4233  OH2 TIP S 176     14.485  79.387  59.276  1.00 36.33      S   O
ATOM  4234  OH2 TIP S 178     -8.133  88.350  22.930  1.00 24.98      S   O
ATOM  4235  OH2 TIP S 179     11.008  89.282  26.933  1.00 26.38      S   O
ATOM  4236  OH2 TIP S 180     29.198  77.232  57.047  1.00 28.34      S   O
ATOM  4237  OH2 TIP S 181     42.985  63.495  21.723  1.00 32.93      S   O
ATOM  4238  OH2 TIP S 182     -2.488  92.239  26.844  1.00 31.41      S   O
ATOM  4239  OH2 TIP S 183     38.070  68.391  49.950  1.00 27.44      S   O
ATOM  4240  OH2 TIP S 184      3.026  87.382  17.697  1.00 24.17      S   O
ATOM  4241  OH2 TIP S 185     32.032  45.265  50.288  1.00 26.40      S   O
ATOM  4242  OH2 TIP S 186     39.904  55.447  42.177  1.00 25.49      S   O
ATOM  4243  OH2 TIP S 187      2.867  70.555  28.600  1.00 25.55      S   O
ATOM  4244  OH2 TIP S 188     28.784  77.898  31.205  1.00 27.78      S   O
ATOM  4245  OH2 TIP S 189      6.525  74.751  39.761  1.00 27.53      S   O
ATOM  4246  OH2 TIP S 190     -6.708  81.142  14.878  1.00 30.15      S   O
ATOM  4247  OH2 TIP S 191     23.949  87.249  38.410  1.00 26.94      S   O
ATOM  4248  OH2 TIP S 192      5.279  83.214  19.647  1.00 23.04      S   O
ATOM  4249  OH2 TIP S 193      7.787  93.915  65.832  1.00 34.56      S   O
ATOM  4250  OH2 TIP S 194     40.056  62.665  49.571  1.00 45.56      S   O
ATOM  4251  OH2 TIP S 195     17.005  83.158  42.309  1.00 26.09      S   O
ATOM  4252  OH2 TIP S 196     39.783  52.482  36.066  1.00 43.89      S   O
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Figure 5VVV

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ATOM  4253  OH2 TIP S 197     21.034  85.408  34.631  1.00 21.18      S   O
ATOM  4254  OH2 TIP S 198     -2.760  93.994  35.518  1.00 32.71      S   O
ATOM  4255  OH2 TIP S 199    -14.876  77.201  34.781  1.00 29.91      S   O
ATOM  4256  OH2 TIP S 200      7.796  94.208  62.630  1.00 34.21      S   O
ATOM  4257  OH2 TIP S 201    -10.407  94.563  54.451  1.00 30.66      S   O
ATOM  4258  OH2 TIP S 202     19.132  85.088  38.251  1.00 26.36      S   O
ATOM  4259  OH2 TIP S 203     46.329  71.427  42.245  1.00 38.45      S   O
ATOM  4260  OH2 TIP S 204     38.151  49.728  42.054  1.00 23.90      S   O
ATOM  4261  OH2 TIP S 205    -16.881  92.357  37.722  1.00 29.19      S   O
ATOM  4262  OH2 TIP S 206      8.018  58.831  39.198  1.00 17.50      S   O
ATOM  4263  OH2 TIP S 207     23.689  77.990  32.612  1.00 37.51      S   O
ATOM  4264  OH2 TIP S 208     30.303  45.065  54.676  1.00 28.16      S   O
ATOM  4265  OH2 TIP S 209     25.161  84.823  52.568  1.00 29.69      S   O
ATOM  4266  OH2 TIP S 210     23.062  78.703  21.684  1.00 26.51      S   O
ATOM  4267  OH2 TIP S 211     26.355  47.512  59.226  1.00 41.38      S   O
ATOM  4268  OH2 TIP S 212     12.364  73.834  56.670  1.00 17.58      S   O
ATOM  4269  OH2 TIP S 213     22.789 101.251  38.634  1.00 36.48      S   O
ATOM  4270  OH2 TIP S 214     30.444  78.274  42.812  1.00 18.27      S   O
ATOM  4271  OH2 TIP S 215     16.714  66.636  43.404  1.00 27.82      S   O
ATOM  4272  OH2 TIP S 216     11.118 110.647  48.883  1.00 41.21      S   O
ATOM  4273  OH2 TIP S 217     11.938  77.223  62.477  1.00 26.78      S   O
ATOM  4274  OH2 TIP S 218     21.348  98.318  46.299  1.00 22.54      S   O
ATOM  4275  OH2 TIP S 219      6.335  90.109  61.055  1.00 30.93      S   O
ATOM  4276  OH2 TIP S 220     16.849  58.092  31.635  1.00 27.78      S   O
ATOM  4277  OH2 TIP S 221    -14.977  98.435  36.110  1.00 29.94      S   O
ATOM  4278  OH2 TIP S 222     32.209  56.644  34.417  1.00 27.61      S   O
ATOM  4279  OH2 TIP S 223     38.616  69.338  19.683  1.00 35.00      S   O
ATOM  4280  OH2 TIP S 224     43.793  66.187  40.980  1.00 28.57      S   O
ATOM  4281  OH2 TIP S 225     25.865  49.291  48.912  1.00 22.19      S   O
ATOM  4282  OH2 TIP S 226     29.493  51.282  39.294  1.00 28.59      S   O
ATOM  4283  OH2 TIP S 227      8.557  68.734  23.715  1.00 32.38      S   O
ATOM  4284  OH2 TIP S 228     35.030  72.215  49.061  1.00 21.47      S   O
ATOM  4285  OH2 TIP S 229     -5.863  84.407  53.693  1.00 32.71      S   O
ATOM  4286  OH2 TIP S 230      8.409  66.822  21.454  1.00 32.17      S   O
ATOM  4287  OH2 TIP S 231     16.090  88.535  25.766  1.00 45.41      S   O
ATOM  4288  OH2 TIP S 232      5.228  66.001  48.372  1.00 33.03      S   O
ATOM  4289  OH2 TIP S 233     22.372  81.334  39.929  1.00 38.56      S   O
ATOM  4290  OH2 TIP S 234    -11.344  82.468  23.312  1.00 32.37      S   O
ATOM  4291  OH2 TIP S 235     -5.663  88.297  52.367  1.00 28.46      S   O
ATOM  4292  OH2 TIP S 236     13.616  74.457  18.786  1.00 42.18      S   O
ATOM  4293  OH2 TIP S 237     25.283  53.133  37.923  1.00 40.56      S   O
ATOM  4294  OH2 TIP S 238      8.026  53.624  54.137  1.00 31.65      S   O
ATOM  4295  OH2 TIP S 239     34.534  62.367  11.800  1.00 31.60      S   O
ATOM  4296  OH2 TIP S 240      1.831  56.099  44.184  1.00 34.48      S   O
ATOM  4297  OH2 TIP S 241     49.497  62.599  26.810  1.00 26.78      S   O
ATOM  4298  OH2 TIP S 242     -4.758  72.368  21.533  1.00 38.11      S   O
ATOM  4299  OH2 TIP S 243     -5.868  83.431  58.623  1.00 34.40      S   O
ATOM  4300  OH2 TIP S 244     29.156  81.797  37.170  1.00 39.60      S   O
ATOM  4301  OH2 TIP S 245     21.609  85.611  37.638  1.00 20.34      S   O
ATOM  4302  OH2 TIP S 246     -4.284  77.490  49.709  1.00 35.30      S   O
ATOM  4303  OH2 TIP S 247     31.807  48.664  61.432  1.00 43.66      S   O
ATOM  4304  OH2 TIP S 248     34.652  80.273  32.759  1.00 35.30      S   O
ATOM  4305  OH2 TIP S 249     -7.767  74.088  33.904  1.00 27.76      S   O
ATOM  4306  OH2 TIP S 250     -0.973  76.943  21.093  1.00 36.81      S   O
ATOM  4307  OH2 TIP S 251     17.520 103.841  50.759  1.00 37.13      S   O
ATOM  4308  OH2 TIP S 252     36.677  59.162  23.943  1.00 39.63      S   O
ATOM  4309  OH2 TIP S 253     -3.985  93.307  65.493  1.00 38.58      S   O
ATOM  4310  OH2 TIP S 254     26.053  53.836  34.851  1.00 37.31      S   O
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Figure 5WWW

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ATOM  4311  OH2 TIP S 255     -7.010  78.156  28.377  1.00 28.40      S   O
ATOM  4312  OH2 TIP S 256      3.198  69.864  24.836  1.00 24.87      S   O
ATOM  4313  OH2 TIP S 257     -2.729  89.793  59.984  1.00 35.90      S   O
ATOM  4314  OH2 TIP S 259     12.874  62.780  21.486  1.00 40.71      S   O
ATOM  4315  OH2 TIP S 260     34.460  53.900  62.259  1.00 37.85      S   O
ATOM  4316  OH2 TIP S 261      8.524  50.114  40.677  1.00 29.93      S   O
ATOM  4317  OH2 TIP S 262     13.534  51.901  52.802  1.00 35.55      S   O
ATOM  4318  OH2 TIP S 263     -5.651  71.332  27.984  1.00 36.22      S   O
ATOM  4319  OH2 TIP S 264     10.884  74.117  37.648  1.00 23.87      S   O
ATOM  4320  OH2 TIP S 265      1.558 105.085  59.290  1.00 30.99      S   O
ATOM  4321  OH2 TIP S 267     22.855  87.241  54.244  1.00 39.85      S   O
ATOM  4322  OH2 TIP S 268     19.606  84.810  44.816  1.00 16.00      S   O
ATOM  4323  OH2 TIP S 269     10.246  57.810  32.854  1.00 25.86      S   O
ATOM  4324  OH2 TIP S 270    -21.599  79.618  39.328  1.00 38.76      S   O
ATOM  4325  OH2 TIP S 271     35.642  69.502  46.091  1.00 25.61      S   O
ATOM  4326  OH2 TIP S 272      7.124  71.606  39.935  1.00 32.52      S   O
ATOM  4327  OH2 TIP S 274     37.219  53.704  29.589  1.00 30.49      S   O
ATOM  4328  OH2 TIP S 275     15.688  71.656  41.660  1.00 35.47      S   O
ATOM  4329  OH2 TIP S 276     18.771  98.089  33.479  1.00 36.76      S   O
ATOM  4330  OH2 TIP S 277     18.891  96.723  59.037  1.00 34.81      S   O
ATOM  4331  OH2 TIP S 279     20.582  96.155  32.990  1.00 36.72      S   O
ATOM  4332  OH2 TIP S 280     38.382  46.507  54.083  1.00 22.09      S   O
ATOM  4333  OH2 TIP S 284     33.499  78.469  29.422  1.00 42.54      S   O
ATOM  4334  OH2 TIP S 285     43.663  56.107  27.511  1.00 34.42      S   O
ATOM  4335  OH2 TIP S 286     35.122  60.670  20.712  1.00 39.38      S   O
ATOM  4336  OH2 TIP S 287     -1.725  96.233  63.363  1.00 35.97      S   O
ATOM  4337  OH2 TIP S 290     18.717  83.949  40.601  1.00 23.89      S   O
ATOM  4338  OH2 TIP S 291     38.772  45.987  46.680  1.00 36.15      S   O
ATOM  4339  OH2 TIP S 292     20.224  69.382  59.695  1.00 29.64      S   O
ATOM  4340  OH2 TIP S 293      8.282  78.199  63.669  1.00 36.59      S   O
ATOM  4341  OH2 TIP S 294     14.047  63.860  59.319  1.00 44.69      S   O
ATOM  4342  OH2 TIP S 297     -5.817  72.739  40.818  1.00 38.14      S   O
ATOM  4343  OH2 TIP S 298     26.321  64.439  12.786  1.00 45.15      S   O
ATOM  4344  OH2 TIP S 299     -6.944 102.099  43.661  1.00 28.91      S   O
ATOM  4345  OH2 TIP S 300     31.982  51.444  38.891  1.00 26.30      S   O
ATOM  4346  OH2 TIP S 301     22.179  61.349  17.217  1.00 28.54      S   O
ATOM  4347  OH2 TIP S 302     11.846  66.672  46.440  1.00 15.33      S   O
ATOM  4348  OH2 TIP S 303     16.579  61.209  61.822  1.00 25.84      S   O
ATOM  4349  OH2 TIP S 304      9.179  61.102  31.089  1.00 35.18      S   O
ATOM  4350  OH2 TIP S 306     43.337  56.983  38.631  1.00 31.17      S   O
ATOM  4351  OH2 TIP S 307     -4.729  79.060  14.954  1.00 29.45      S   O
ATOM  4352  OH2 TIP S 309      3.264  96.531  34.343  1.00 35.87      S   O
ATOM  4353  OH2 TIP S 310     33.597  56.115  32.020  1.00 38.28      S   O
ATOM  4354  OH2 TIP S 312     21.131  84.199  42.642  1.00 16.36      S   O
ATOM  4355  OH2 TIP S 314     13.289  90.298  22.035  1.00 37.86      S   O
ATOM  4356  OH2 TIP S 315    -21.318  88.597  32.650  1.00 31.68      S   O
ATOM  4357  OH2 TIP S 316      0.324  97.812  61.903  1.00 28.65      S   O
ATOM  4358  OH2 TIP S 317     15.681  48.773  53.561  1.00 32.11      S   O
ATOM  4359  OH2 TIP S 318      6.414  66.203  28.644  1.00 45.39      S   O
ATOM  4360  OH2 TIP S 320     21.877  45.789  57.051  1.00 37.88      S   O
ATOM  4361  OH2 TIP S 325     33.257  76.751  48.828  1.00 36.69      S   O
ATOM  4362  OH2 TIP S 326     -1.477  99.714  39.504  1.00 31.96      S   O
ATOM  4363  OH2 TIP S 327      7.083 107.442  40.232  1.00 34.50      S   O
ATOM  4364  OH2 TIP S 328     19.455  81.284  39.450  1.00 31.13      S   O
ATOM  4365  OH2 TIP S 330     18.928  59.678  27.698  1.00 23.64      S   O
ATOM  4366  OH2 TIP S 333      2.949  68.265  43.594  1.00 46.66      S   O
ATOM  4367  OH2 TIP S 334     -8.138 104.339  45.239  1.00 36.83      S   O
ATOM  4368  OH2 TIP S 336      3.891  58.458  48.159  1.00 40.09      S   O
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Figure 5XXX

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ATOM  4369  OH2 TIP S 339    -11.491  79.098  22.692  1.00 31.58      S   O
ATOM  4370  OH2 TIP S 342     -3.605  77.350  56.479  1.00 33.40      S   O
ATOM  4371  OH2 TIP S 345     48.945  64.149  23.906  1.00 33.98      S   O
ATOM  4372  OH2 TIP S 348     17.597  50.879  59.000  1.00 46.70      S   O
ATOM  4373  OH2 TIP S 349    -19.548  99.216  33.850  1.00 31.30      S   O
ATOM  4374  OH2 TIP S 350     11.566  66.969  42.047  1.00 25.33      S   O
ATOM  4375  OH2 TIP S 353     24.674  43.379  42.738  1.00 46.49      S   O
ATOM  4376  OH2 TIP S 354     20.654  78.836  55.418  1.00 19.53      S   O
ATOM  4377  OH2 TIP S 357     17.254  91.782  60.031  1.00 23.92      S   O
ATOM  4378  OH2 TIP S 358      9.923  67.047  44.491  1.00 20.59      S   O
ATOM  4379  OH2 TIP S 359     36.952  66.998  45.661  1.00 21.28      S   O
ATOM  4380  OH2 TIP S 360     15.012  70.447  58.501  1.00 20.49      S   O
ATOM  4381  OH2 TIP S 361     38.560  66.828  47.799  1.00 18.16      S   O
ATOM  4382  OH2 TIP S 362     12.567  70.351  43.331  1.00 21.60      S   O
ATOM  4383  OH2 TIP S 363     10.275  70.909  59.173  1.00 20.25      S   O
ATOM  4384  OH2 TIP S 365     -8.636  80.604  29.420  1.00 20.84      S   O
ATOM  4385  OH2 TIP S 366     27.535  82.312  43.508  1.00 25.30      S   O
ATOM  4386  OH2 TIP S 367     17.257  86.397  26.338  1.00 29.08      S   O
ATOM  4387  OH2 TIP S 368      4.358  55.280  44.796  1.00 40.14      S   O
ATOM  4388  OH2 TIP S 369      8.463  83.561  21.334  1.00 22.41      S   O
ATOM  4389  OH2 TIP S 370     -8.086  97.612  37.816  1.00 25.46      S   O
ATOM  4390  OH2 TIP S 371     12.843  74.928  39.116  1.00 31.70      S   O
ATOM  4391  OH2 TIP S 372      8.347  72.232  57.105  1.00 25.70      S   O
ATOM  4392  OH2 TIP S 373     -3.834 109.911  52.412  1.00 25.46      S   O
ATOM  4393  OH2 TIP S 374     38.734  67.042  43.751  1.00 25.21      S   O
ATOM  4394  OH2 TIP S 375     20.952  90.132  33.041  1.00 26.25      S   O
ATOM  4395  OH2 TIP S 376     21.122  98.404  49.083  1.00 21.33      S   O
ATOM  4396  OH2 TIP S 377    -12.795  97.771  42.948  1.00 27.19      S   O
ATOM  4397  OH2 TIP S 378     24.316  79.549  28.534  1.00 25.40      S   O
ATOM  4398  OH2 TIP S 379     27.736  88.375  45.434  1.00 29.24      S   O
ATOM  4399  OH2 TIP S 380      8.225  59.683  36.172  1.00 24.77      S   O
ATOM  4400  OH2 TIP S 381     37.450  53.227  35.003  1.00 32.48      S   O
ATOM  4401  OH2 TIP S 382    -10.586  84.900  22.199  1.00 30.47      S   O
ATOM  4402  OH2 TIP S 383    -15.137  95.854  40.707  1.00 25.76      S   O
ATOM  4403  OH2 TIP S 384     16.777  65.477  62.229  1.00 26.46      S   O
ATOM  4404  OH2 TIP S 385     28.839  86.168  50.617  1.00 33.26      S   O
ATOM  4405  OH2 TIP S 386     17.382  84.892  57.199  1.00 22.87      S   O
ATOM  4406  OH2 TIP S 387     27.000  52.190  62.926  1.00 27.15      S   O
ATOM  4407  OH2 TIP S 388     31.661  79.835  35.615  1.00 28.03      S   O
ATOM  4408  OH2 TIP S 389     -4.676  84.758  48.894  1.00 31.68      S   O
ATOM  4409  OH2 TIP S 390     -5.662  91.557  50.040  1.00 31.19      S   O
ATOM  4410  OH2 TIP S 391     23.487  83.965  44.473  1.00 28.65      S   O
ATOM  4411  OH2 TIP S 392     -6.441  88.875  58.175  1.00 33.33      S   O
ATOM  4412  OH2 TIP S 393      7.603  93.526  36.250  1.00 30.57      S   O
ATOM  4413  OH2 TIP S 394     49.203  72.825  26.301  1.00 24.46      S   O
ATOM  4414  OH2 TIP S 395     28.479  61.371  62.617  1.00 32.12      S   O
ATOM  4415  OH2 TIP S 397     -9.168  83.076  17.253  1.00 25.74      S   O
ATOM  4416  OH2 TIP S 398     16.075  88.965  63.990  1.00 30.49      S   O
ATOM  4417  OH2 TIP S 400     13.310  95.842  67.259  1.00 29.76      S   O
ATOM  4418  OH2 TIP S 401      5.918  66.938  33.592  1.00 31.14      S   O
ATOM  4419  OH2 TIP S 402      0.155 106.248  55.777  1.00 32.60      S   O
ATOM  4420  OH2 TIP S 403      6.110  92.248  62.655  1.00 27.95      S   O
ATOM  4421  OH2 TIP S 404      2.233 103.880  39.763  1.00 31.52      S   O
ATOM  4422  OH2 TIP S 405     25.694  98.715  48.972  1.00 29.93      S   O
ATOM  4423  OH2 TIP S 406     10.674  73.231  60.407  1.00 31.34      S   O
ATOM  4424  OH2 TIP S 409     51.882  66.157  29.120  1.00 26.96      S   O
ATOM  4425  OH2 TIP S 410      6.325  68.647  46.053  1.00 34.29      S   O
ATOM  4426  OH2 TIP S 412     39.391  64.285  54.825  1.00 28.64      S   O
```

Figure 5YYY

```
ATOM  4427 OH2 TIP S 413     -2.620  73.079  47.858  1.00 31.55      S   O
ATOM  4428 OH2 TIP S 414     32.879  78.973  43.464  1.00 29.58      S   O
ATOM  4429 OH2 TIP S 415    -15.016  96.572  33.202  1.00 45.53      S   O
ATOM  4430 OH2 TIP S 416     39.377  75.743  32.551  1.00 30.17      S   O
ATOM  4431 OH2 TIP S 417     31.294  47.074  59.585  1.00 32.29      S   O
ATOM  4432 OH2 TIP S 418     20.908  99.085  60.072  1.00 33.84      S   O
ATOM  4433 OH2 TIP S 421     16.227  75.089  58.255  1.00 34.63      S   O
ATOM  4434 OH2 TIP S 423      9.515  68.766  41.162  1.00 31.09      S   O
ATOM  4435 OH2 TIP S 424     24.057  90.877  41.184  1.00 32.57      S   O
ATOM  4436 OH2 TIP S 425    -23.421  85.321  34.874  1.00 40.73      S   O
ATOM  4437 OH2 TIP S 426     -6.600  85.509  60.637  1.00 36.33      S   O
ATOM  4438 OH2 TIP S 429     18.068  74.274  39.152  1.00 28.30      S   O
ATOM  4439 OH2 TIP S 430      0.216  72.088  29.280  1.00 34.77      S   O
ATOM  4440 OH2 TIP S 431     24.237  97.970  52.510  1.00 40.38      S   O
ATOM  4441 OH2 TIP S 433     16.496  61.776  20.380  1.00 31.74      S   O
ATOM  4442 OH2 TIP S 434     23.656  81.140  23.402  1.00 39.14      S   O
ATOM  4443 OH2 TIP S 435     45.512  70.376  23.767  1.00 38.06      S   O
ATOM  4444 OH2 TIP S 436      5.133  69.622  42.446  1.00 33.04      S   O
ATOM  4445 OH2 TIP S 440     23.692  79.457  34.661  1.00 40.65      S   O
ATOM  4446 OH2 TIP S 443     15.889  73.328  39.832  1.00 29.37      S   O
ATOM  4447 OH2 TIP S 444     -8.745  70.532  28.410  1.00 33.62      S   O
ATOM  4448 OH2 TIP S 446     32.260  78.506  13.999  1.00 45.13      S   O
ATOM  4449 OH2 TIP S 448     39.242  48.079  43.803  1.00 33.38      S   O
ATOM  4450 OH2 TIP S 449     34.559  75.768  22.405  1.00 31.84      S   O
ATOM  4451 OH2 TIP S 450     17.344  71.627  57.656  1.00 30.16      S   O
ATOM  4452 OH2 TIP S 453     17.850  55.704  64.074  1.00 41.95      S   O
ATOM  4453 OH2 TIP S 454     12.673  87.630  65.105  1.00 36.77      S   O
ATOM  4454 OH2 TIP S 455     18.393  73.689  58.998  1.00 35.69      S   O
ATOM  4455 OH2 TIP S 457     31.350  80.284  54.849  1.00 32.98      S   O
ATOM  4456 OH2 TIP S 459     31.948  64.117  63.134  1.00 33.16      S   O
ATOM  4457 OH2 TIP S 461     25.883  44.584  58.922  1.00 26.81      S   O
ATOM  4458 OH2 TIP S 462     15.411  75.744  38.970  1.00 38.18      S   O
ATOM  4459 OH2 TIP S 465     -6.694  85.996  51.462  1.00 39.03      S   O
ATOM  4460 OH2 TIP S 467     22.428  74.991  56.119  1.00 48.69      S   O
ATOM  4461 OH2 TIP S 472      7.409  68.343  43.765  1.00 40.63      S   O
ATOM  4462 OH2 TIP S 477      3.696  81.760  15.765  1.00 41.18      S   O
ATOM  4463 OH2 TIP S 478     36.353  75.696  51.865  1.00 40.40      S   O
ATOM  4464 OH2 TIP S 479     45.063  73.009  39.613  1.00 30.28      S   O
ATOM  4465 OH2 TIP S 480     35.167  68.155  64.949  1.00 36.43      S   O
ATOM  4466 OH2 TIP S 481     16.895  81.810  19.179  1.00 26.87      S   O
ATOM  4467 OH2 TIP S 482      9.338  64.581  19.670  1.00 47.45      S   O
ATOM  4468 OH2 TIP S 486     -4.142  97.143  32.076  1.00 40.89      S   O
ATOM  4469 OH2 TIP S 492      8.626 110.626  48.140  1.00 38.81      S   O
ATOM  4470 OH2 TIP S 493     10.344  52.396  54.552  1.00 40.72      S   O
ATOM  4471 OH2 TIP S 504     -6.927  90.936  52.736  1.00 32.58      S   O
ATOM  4472 OH2 TIP S 506     25.842  56.111  26.259  1.00 44.04      S   O
ATOM  4473 OH2 TIP S 511    -18.765  81.021  30.433  1.00 43.07      S   O
ATOM  4474 OH2 TIP S 514    -10.951  95.897  30.634  1.00 35.08      S   O
ATOM  4475 OH2 TIP S 515     18.239  91.555  29.988  1.00 35.01      S   O
ATOM  4476 OH2 TIP S 518     11.487  71.453  37.559  1.00 30.35      S   O
ATOM  4477 OH2 TIP S 519     -5.621  94.181  63.866  1.00 38.29      S   O
ATOM  4478 OH2 TIP S 522    -22.715  82.630  39.313  1.00 37.68      S   O
ATOM  4479 OH2 TIP S 523     13.832  92.634  28.634  1.00 42.35      S   O
ATOM  4480 OH2 TIP S 526     38.684  51.235  34.304  1.00 47.63      S   O
ATOM  4481 OH2 TIP S 528     36.575  81.337  36.652  1.00 30.20      S   O
ATOM  4482 OH2 TIP S 529     19.003  94.626  60.449  1.00 33.39      S   O
ATOM  4483 OH2 TIP S 532     45.213  64.758  44.484  1.00 43.40      S   O
ATOM  4484 OH2 TIP S 548     27.913  76.880  61.466  1.00 39.53      S   O
```

Figure 5ZZZ

```
ATOM   4485  OH2 TIP S 550     -7.794  83.071  55.228  1.00 36.58      S    O
ATOM   4486  OH2 TIP S 551      6.856  87.791  20.410  1.00 45.36      S    O
ATOM   4487  OH2 TIP S 553     20.954  56.587  35.076  1.00 46.06      S    O
ATOM   4488  OH2 TIP S 559      6.709  95.476  37.577  1.00 37.67      S    O
ATOM   4489  OH2 TIP S 561     -5.111  70.585  43.095  1.00 36.29      S    O
ATOM   4490  OH2 TIP S 563     33.592  49.188  39.439  1.00 38.90      S    O
ATOM   4491  OH2 TIP S 567     24.268  93.456  38.866  1.00 41.73      S    O
ATOM   4492  OH2 TIP S 568     38.145  71.373  18.079  1.00 45.93      S    O
ATOM   4493  OH2 TIP S 570     10.042 104.897  57.893  1.00 35.94      S    O
ATOM   4494  OH2 TIP S 579      2.980  71.667  46.083  1.00 31.08      S    O
ATOM   4495  OH2 TIP S 588     42.992  48.494  46.292  1.00 42.53      S    O
ATOM   4496  OH2 TIP S 592      7.979 101.256  62.776  1.00 43.56      S    O
ATOM   4497  OH2 TIP S 596     40.729  51.604  40.374  1.00 44.86      S    O
ATOM   4498  OH2 TIP S 608     22.066  82.819  34.739  1.00 44.19      S    O
ATOM   4499  OH2 TIP S 612     23.253  56.890  32.646  1.00 37.91      S    O
ATOM   4500  OH2 TIP S 613     -4.126  71.281  39.257  1.00 40.53      S    O
ATOM   4501  OH2 TIP S 640     21.624 103.517  40.110  1.00 37.27      S    O
ATOM   4502  OH2 TIP S 648      5.614  70.703  52.258  1.00 52.65      S    O
ATOM   4503  OH2 TIP S 650     43.903  58.744  50.765  1.00 33.40      S    O
ATOM   4504  OH2 TIP S 655     -8.816  78.637  48.006  1.00 40.13      S    O
ATOM   4505  OH2 TIP S 656     -5.358  78.170  23.376  1.00 32.77      S    O
ATOM   4506  OH2 TIP S 657      3.160  70.067  31.591  1.00 35.22      S    O
ATOM   4507  OH2 TIP S 658     25.185  73.553  62.291  1.00 39.81      S    O
END
```

Figure 6A

```
REMARK Created by MOLEMAN V. 991230/7.3 at Tue Dec 10 19:34:52 2002 for kemitl
REMARK MoleMan PDB file
REMARK Created by MOLEMAN V. 961218/7.2.5 at Tue Mar 28 15:09:11 2000 for kemitl
REMARK MoleMan PDB file
REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 1.86 A
REMARK starting r= 0.2208 free_r= 0.2457
REMARK final   r= 0.2055 free_r= 0.2376
REMARK B rmsd for bonded mainchain atoms=  1.483  target= 1.5
REMARK B rmsd for bonded sidechain atoms=  2.506  target= 2.0
REMARK B rmsd for angle mainchain atoms=  2.042  target= 2.0
REMARK B rmsd for angle sidechain atoms=  3.617  target= 2.5
REMARK wa= 1.64705
REMARK rweight=6.377507E-02
REMARK target= mlf  steps= 50
REMARK sg= P2(1)2(1)2(1) a= 61.41 b= 76.31 c= 108.92 alpha= 90 beta= 90 gamma= 90
REMARK parameter file 1  : MSI_CNX_TOPPAR:protein_rep.param
REMARK parameter file 2  : MSI_CNX_TOPPAR:water_rep.param
REMARK parameter file 3  : inh.par
REMARK parameter file 4  : gld.par
REMARK molecular structure file: generate_easy.psf
REMARK input coordinates: bgroup.pdb
REMARK reflection file= muri_1.8.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.86
REMARK initial B-factor correction applied to fobs :
REMARK   B11=   0.497 B22=   1.667 B33=  -2.164
REMARK   B12=   0.000 B13=   0.000 B23=   0.000
REMARK B-factor correction applied to coordinate array B:    1.176
REMARK bulk solvent: (Mask) density level= 0.365438 e/A^3, B-factor= 33.2255 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range:    43743 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):  3410 (  7.8 % )
REMARK number of reflections rejected:                           0 (  0.0 % )
REMARK total number of reflections used:                     40333 ( 92.2 % )
REMARK number of reflections in working set:                 38313 ( 87.6 % )
REMARK number of reflections in test set:                    2020 (  4.6 % )
REMARK FILENAME="bindividual.pdb"
REMARK DATE:Mar-24-2000  16:16:02      created by user: kemitl
REMARK Written by CNX VERSION:2000
CRYST1  61.410  76.310 108.920 90.00  90.00  90.00 P212121      1
ORIGX1     1.000000 0.000000 0.000000       0.00000
ORIGX2     0.000000 1.000000 0.000000       0.00000
ORIGX3     0.000000 0.000000 1.000000       0.00000
SCALE1     0.016284 0.000000 0.000000       0.00000
SCALE2     0.000000 0.013104 0.000000       0.00000
SCALE3     0.000000 0.000000 0.009181       0.00000
ATOM     1  CB  MET A  1     30.124  48.907  56.585  1.00 22.42     A   C
ATOM     2  CG  MET A  1     30.702  50.302  56.333  1.00 25.22     A   C
ATOM     3  SD  MET A  1     31.489  51.055  57.785  1.00 28.98     A   S
ATOM     4  CE  MET A  1     32.951  49.983  58.010  1.00 26.14     A   C
ATOM     5  C   MET A  1     27.890  49.690  57.412  1.00 19.35     A   C
ATOM     6  O   MET A  1     27.114  49.386  56.503  1.00 20.53     A   O
ATOM     7  N   MET A  1     28.658  47.421  57.925  1.00 18.28     A   N
ATOM     8  CA  MET A  1     29.106  48.829  57.729  1.00 20.61     A   C
ATOM     9  N   LYS A  2     27.729  50.760  58.178  1.00 18.84     A   N
ATOM    10  CA  LYS A  2     26.605  51.666  58.005  1.00 19.29     A   C
```

Figure 6B

```
ATOM   11 CB  LYS A  2     25.834  51.769  59.316  1.00 18.82    A   C
ATOM   12 CG  LYS A  2     24.636  52.702  59.295  1.00 20.09    A   C
ATOM   13 CD  LYS A  2     24.005  52.752  60.674  1.00 22.85    A   C
ATOM   14 CE  LYS A  2     22.697  53.523  60.676  1.00 22.98    A   C
ATOM   15 NZ  LYS A  2     22.078  53.501  62.033  1.00 22.51    A   N
ATOM   16 C   LYS A  2     27.131  53.031  57.588  1.00 17.25    A   C
ATOM   17 O   LYS A  2     27.980  53.616  58.265  1.00 16.44    A   O
ATOM   18 N   ILE A  3     26.630  53.533  56.464  1.00 17.70    A   N
ATOM   19 CA  ILE A  3     27.075  54.824  55.968  1.00 14.65    A   C
ATOM   20 CB  ILE A  3     28.001  54.647  54.738  1.00 16.82    A   C
ATOM   21 CG2 ILE A  3     29.214  53.807  55.121  1.00 17.12    A   C
ATOM   22 CG1 ILE A  3     27.252  53.971  53.593  1.00 17.27    A   C
ATOM   23 CD1 ILE A  3     26.697  54.929  52.583  1.00 20.09    A   C
ATOM   24 C   ILE A  3     25.925  55.758  55.617  1.00 14.64    A   C
ATOM   25 O   ILE A  3     24.752  55.377  55.639  1.00 14.39    A   O
ATOM   26 N   GLY A  4     26.269  57.001  55.322  1.00 13.89    A   N
ATOM   27 CA  GLY A  4     25.244  57.956  54.961  1.00 14.96    A   C
ATOM   28 C   GLY A  4     25.500  58.490  53.569  1.00 13.26    A   C
ATOM   29 O   GLY A  4     26.634  58.453  53.081  1.00 11.89    A   O
ATOM   30 N   VAL A  5     24.439  58.954  52.917  1.00 11.22    A   N
ATOM   31 CA  VAL A  5     24.549  59.541  51.592  1.00 10.79    A   C
ATOM   32 CB  VAL A  5     23.964  58.625  50.500  1.00 14.07    A   C
ATOM   33 CG1 VAL A  5     23.918  59.363  49.169  1.00 12.77    A   C
ATOM   34 CG2 VAL A  5     24.828  57.385  50.352  1.00 12.02    A   C
ATOM   35 C   VAL A  5     23.771  60.848  51.643  1.00 11.63    A   C
ATOM   36 O   VAL A  5     22.596  60.872  52.020  1.00 12.22    A   O
ATOM   37 N   PHE A  6     24.445  61.932  51.287  1.00 11.51    A   N
ATOM   38 CA  PHE A  6     23.848  63.256  51.302  1.00 13.29    A   C
ATOM   39 CB  PHE A  6     24.674  64.182  52.203  1.00 13.43    A   C
ATOM   40 CG  PHE A  6     24.252  65.620  52.143  1.00 14.85    A   C
ATOM   41 CD1 PHE A  6     22.937  65.981  52.418  1.00 16.29    A   C
ATOM   42 CD2 PHE A  6     25.164  66.612  51.800  1.00 15.26    A   C
ATOM   43 CE1 PHE A  6     22.530  67.317  52.350  1.00 17.43    A   C
ATOM   44 CE2 PHE A  6     24.770  67.954  51.728  1.00 17.55    A   C
ATOM   45 CZ  PHE A  6     23.450  68.305  52.003  1.00 18.07    A   C
ATOM   46 C   PHE A  6     23.725  63.887  49.920  1.00 12.87    A   C
ATOM   47 O   PHE A  6     24.641  63.806  49.102  1.00 14.09    A   O
ATOM   48 N   ASP A  7     22.583  64.519  49.674  1.00 11.45    A   N
ATOM   49 CA  ASP A  7     22.331  65.212  48.418  1.00 12.53    A   C
ATOM   50 CB  ASP A  7     21.749  64.263  47.363  1.00 11.52    A   C
ATOM   51 CG  ASP A  7     21.491  64.959  46.035  1.00 10.71    A   C
ATOM   52 OD1 ASP A  7     22.444  65.525  45.457  1.00 12.13    A   O
ATOM   53 OD2 ASP A  7     20.332  64.944  45.571  1.00 11.62    A   O
ATOM   54 C   ASP A  7     21.353  66.350  48.670  1.00 10.34    A   C
ATOM   55 O   ASP A  7     20.714  66.410  49.716  1.00 12.06    A   O
ATOM   56 N   SER A  8     21.245  67.262  47.713  1.00 12.07    A   N
ATOM   57 CA  SER A  8     20.330  68.387  47.856  1.00 12.93    A   C
ATOM   58 CB  SER A  8     20.595  69.417  46.756  1.00 12.10    A   C
ATOM   59 OG  SER A  8     20.364  68.857  45.474  1.00 10.24    A   O
ATOM   60 C   SER A  8     18.874  67.909  47.783  1.00 13.34    A   C
ATOM   61 O   SER A  8     17.957  68.609  48.217  1.00 14.16    A   O
ATOM   62 N   GLY A  9     18.667  66.709  47.250  1.00 13.06    A   N
ATOM   63 CA  GLY A  9     17.319  66.182  47.143  1.00 12.56    A   C
ATOM   64 C   GLY A  9     17.253  64.728  46.721  1.00 13.45    A   C
ATOM   65 O   GLY A  9     17.886  63.861  47.329  1.00 13.56    A   O
ATOM   66 N   VAL A 10     16.484  64.460  45.671  1.00 12.87    A   N
ATOM   67 CA  VAL A 10     16.323  63.104  45.159  1.00 12.62    A   C
ATOM   68 CB  VAL A 10     14.916  62.935  44.552  1.00 12.47    A   C
```

Figure 6C

```
ATOM   69 CG1 VAL A 10    14.715 63.955 43.453 1.00 11.29    A   C
ATOM   70 CG2 VAL A 10    14.720 61.521 44.031 1.00 12.71    A   C
ATOM   71 C  VAL A 10     17.372 62.785 44.095 1.00 12.55    A   C
ATOM   72 O  VAL A 10     17.586 61.624 43.749 1.00 11.19    A   O
ATOM   73 N  GLY A 11     18.020 63.823 43.575 1.00 12.78    A   N
ATOM   74 CA GLY A 11     19.032 63.623 42.548 1.00 10.57    A   C
ATOM   75 C  GLY A 11     20.039 62.536 42.884 1.00 12.63    A   C
ATOM   76 O  GLY A 11     20.376 61.696 42.035 1.00 12.33    A   O
ATOM   77 N  GLY A 12     20.514 62.560 44.126 1.00 12.27    A   N
ATOM   78 CA GLY A 12     21.488 61.589 44.597 1.00 13.34    A   C
ATOM   79 C  GLY A 12     21.125 60.142 44.331 1.00 12.55    A   C
ATOM   80 O  GLY A 12     21.963 59.252 44.496 1.00 12.07    A   O
ATOM   81 N  PHE A 13     19.877 59.894 43.938 1.00 11.81    A   N
ATOM   82 CA PHE A 13     19.447 58.534 43.619 1.00 12.39    A   C
ATOM   83 CB PHE A 13     18.009 58.515 43.081 1.00 13.67    A   C
ATOM   84 CG PHE A 13     16.947 58.401 44.148 1.00 13.33    A   C
ATOM   85 CD1 PHE A 13    15.671 57.955 43.816 1.00 14.75    A   C
ATOM   86 CD2 PHE A 13    17.215 58.740 45.470 1.00 13.91    A   C
ATOM   87 CE1 PHE A 13    14.667 57.846 44.790 1.00 18.10    A   C
ATOM   88 CE2 PHE A 13    16.221 58.635 46.454 1.00 15.28    A   C
ATOM   89 CZ PHE A 13     14.943 58.186 46.112 1.00 13.91    A   C
ATOM   90 C  PHE A 13     20.361 57.940 42.547 1.00 13.92    A   C
ATOM   91 O  PHE A 13     20.630 56.737 42.551 1.00 12.12    A   O
ATOM   92 N  SER A 14     20.827 58.781 41.625 1.00 13.26    A   N
ATOM   93 CA SER A 14     21.690 58.304 40.547 1.00 13.42    A   C
ATOM   94 CB SER A 14     21.967 59.423 39.525 1.00 13.96    A   C
ATOM   95 OG SER A 14     22.695 60.504 40.071 1.00 12.20    A   O
ATOM   96 C  SER A 14     22.992 57.730 41.092 1.00 13.28    A   C
ATOM   97 O  SER A 14     23.559 56.805 40.509 1.00 14.54    A   O
ATOM   98 N  VAL A 15     23.458 58.270 42.214 1.00 10.88    A   N
ATOM   99 CA VAL A 15     24.674 57.777 42.846 1.00 11.83    A   C
ATOM   100 CB VAL A 15    25.338 58.859 43.730 1.00 11.43    A   C
ATOM   101 CG1 VAL A 15   26.452 58.243 44.580 1.00 10.44    A   C
ATOM   102 CG2 VAL A 15   25.909 59.960 42.849 1.00 11.65    A   C
ATOM   103 C  VAL A 15    24.333 56.566 43.709 1.00 13.82    A   C
ATOM   104 O  VAL A 15    25.068 55.579 43.727 1.00 13.72    A   O
ATOM   105 N  LEU A 16    23.199 56.635 44.400 1.00 13.39    A   N
ATOM   106 CA LEU A 16    22.767 55.546 45.264 1.00 14.00    A   C
ATOM   107 CB LEU A 16    21.479 55.937 45.993 1.00 11.47    A   C
ATOM   108 CG LEU A 16    20.947 54.898 46.991 1.00 14.59    A   C
ATOM   109 CD1 LEU A 16   22.049 54.511 47.980 1.00 13.56    A   C
ATOM   110 CD2 LEU A 16   19.743 55.477 47.733 1.00 10.24    A   C
ATOM   111 C  LEU A 16    22.562 54.246 44.486 1.00 14.34    A   C
ATOM   112 O  LEU A 16    22.879 53.162 44.980 1.00 13.30    A   O
ATOM   113 N  LYS A 17    22.044 54.356 43.267 1.00 14.05    A   N
ATOM   114 CA LYS A 17    21.822 53.176 42.438 1.00 16.52    A   C
ATOM   115 CB LYS A 17    21.229 53.584 41.087 1.00 16.99    A   C
ATOM   116 CG LYS A 17    21.051 52.424 40.114 1.00 21.73    A   C
ATOM   117 CD LYS A 17    20.461 52.893 38.802 1.00 24.05    A   C
ATOM   118 CE LYS A 17    20.298 51.729 37.833 1.00 27.52    A   C
ATOM   119 NZ LYS A 17    19.805 52.178 36.505 1.00 24.97    A   N
ATOM   120 C  LYS A 17    23.136 52.423 42.220 1.00 17.90    A   C
ATOM   121 O  LYS A 17    23.194 51.193 42.319 1.00 16.07    A   O
ATOM   122 N  SER A 18    24.193 53.171 41.931 1.00 16.04    A   N
ATOM   123 CA SER A 18    25.508 52.582 41.691 1.00 17.22    A   C
ATOM   124 CB SER A 18    26.494 53.663 41.248 1.00 16.33    A   C
ATOM   125 OG SER A 18    26.080 54.255 40.034 1.00 15.13    A   O
ATOM   126 C  SER A 18    26.033 51.900 42.944 1.00 16.33    A   C
```

Figure 6D

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ATOM   127  O   SER A  18      26.579  50.795  42.885  1.00 14.32      A   O
ATOM   128  N   LEU A  19      25.863  52.577  44.075  1.00 13.38      A   N
ATOM   129  CA  LEU A  19      26.301  52.072  45.367  1.00 14.03      A   C
ATOM   130  CB  LEU A  19      26.009  53.102  46.456  1.00 11.70      A   C
ATOM   131  CG  LEU A  19      26.748  54.435  46.350  1.00 12.66      A   C
ATOM   132  CD1 LEU A  19      26.284  55.365  47.471  1.00 13.24      A   C
ATOM   133  CD2 LEU A  19      28.248  54.185  46.442  1.00 11.34      A   C
ATOM   134  C   LEU A  19      25.605  50.771  45.720  1.00 15.80      A   C
ATOM   135  O   LEU A  19      26.240  49.831  46.195  1.00 14.57      A   O
ATOM   136  N   LEU A  20      24.294  50.727  45.496  1.00 15.82      A   N
ATOM   137  CA  LEU A  20      23.510  49.540  45.793  1.00 18.19      A   C
ATOM   138  CB  LEU A  20      22.026  49.807  45.515  1.00 16.40      A   C
ATOM   139  CG  LEU A  20      21.346  50.798  46.473  1.00 16.62      A   C
ATOM   140  CD1 LEU A  20      19.949  51.156  45.974  1.00 16.53      A   C
ATOM   141  CD2 LEU A  20      21.279  50.176  47.867  1.00 16.65      A   C
ATOM   142  C   LEU A  20      23.983  48.330  44.988  1.00 20.92      A   C
ATOM   143  O   LEU A  20      24.179  47.247  45.538  1.00 20.94      A   O
ATOM   144  N   LYS A  21      24.169  48.511  43.687  1.00 20.60      A   N
ATOM   145  CA  LYS A  21      24.612  47.406  42.847  1.00 22.68      A   C
ATOM   146  CB  LYS A  21      24.656  47.840  41.380  1.00 21.65      A   C
ATOM   147  CG  LYS A  21      24.973  46.699  40.426  1.00 26.15      A   C
ATOM   148  CD  LYS A  21      25.083  47.169  38.988  1.00 29.67      A   C
ATOM   149  CE  LYS A  21      25.506  46.017  38.078  1.00 34.31      A   C
ATOM   150  NZ  LYS A  21      25.776  46.469  36.684  1.00 32.80      A   N
ATOM   151  C   LYS A  21      25.978  46.863  43.263  1.00 21.58      A   C
ATOM   152  O   LYS A  21      26.214  45.654  43.208  1.00 23.12      A   O
ATOM   153  N   ALA A  22      26.868  47.753  43.692  1.00 19.68      A   N
ATOM   154  CA  ALA A  22      28.216  47.360  44.093  1.00 19.96      A   C
ATOM   155  CB  ALA A  22      29.131  48.585  44.080  1.00 14.81      A   C
ATOM   156  C   ALA A  22      28.317  46.635  45.446  1.00 20.35      A   C
ATOM   157  O   ALA A  22      29.402  46.199  45.839  1.00 21.92      A   O
ATOM   158  N   ARG A  23      27.198  46.509  46.154  1.00 20.50      A   N
ATOM   159  CA  ARG A  23      27.187  45.821  47.444  1.00 21.19      A   C
ATOM   160  CB  ARG A  23      27.205  44.307  47.230  1.00 23.64      A   C
ATOM   161  CG  ARG A  23      25.965  43.756  46.553  1.00 24.47      A   C
ATOM   162  CD  ARG A  23      26.093  42.252  46.372  1.00 30.28      A   C
ATOM   163  NE  ARG A  23      26.418  41.582  47.630  1.00 30.56      A   N
ATOM   164  CZ  ARG A  23      26.768  40.302  47.727  1.00 32.70      A   C
ATOM   165  NH1 ARG A  23      26.838  39.549  46.636  1.00 32.50      A   N
ATOM   166  NH2 ARG A  23      27.054  39.776  48.914  1.00 28.66      A   N
ATOM   167  C   ARG A  23      28.379  46.216  48.302  1.00 21.73      A   C
ATOM   168  O   ARG A  23      29.149  45.365  48.759  1.00 20.27      A   O
ATOM   169  N   LEU A  24      28.522  47.512  48.527  1.00 17.52      A   N
ATOM   170  CA  LEU A  24      29.624  48.018  49.317  1.00 21.03      A   C
ATOM   171  CB  LEU A  24      30.080  49.366  48.757  1.00 20.25      A   C
ATOM   172  CG  LEU A  24      30.478  49.366  47.282  1.00 22.97      A   C
ATOM   173  CD1 LEU A  24      30.723  50.797  46.810  1.00 22.12      A   C
ATOM   174  CD2 LEU A  24      31.723  48.510  47.094  1.00 21.35      A   C
ATOM   175  C   LEU A  24      29.239  48.184  50.776  1.00 21.90      A   C
ATOM   176  O   LEU A  24      30.079  48.032  51.663  1.00 23.97      A   O
ATOM   177  N   PHE A  25      27.968  48.483  51.028  1.00 20.73      A   N
ATOM   178  CA  PHE A  25      27.517  48.710  52.396  1.00 21.16      A   C
ATOM   179  CB  PHE A  25      27.290  50.207  52.609  1.00 19.75      A   C
ATOM   180  CG  PHE A  25      28.416  51.062  52.101  1.00 19.70      A   C
ATOM   181  CD1 PHE A  25      28.249  51.854  50.967  1.00 20.65      A   C
ATOM   182  CD2 PHE A  25      29.648  51.065  52.748  1.00 19.59      A   C
ATOM   183  CE1 PHE A  25      29.294  52.641  50.483  1.00 20.02      A   C
ATOM   184  CE2 PHE A  25      30.701  51.846  52.276  1.00 20.92      A   C
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Figure 6E

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ATOM   185 CZ  PHE A 25     30.522  52.639  51.137  1.00 19.72    A   C
ATOM   186 C   PHE A 25     26.259  47.940  52.773  1.00 18.19    A   C
ATOM   187 O   PHE A 25     25.387  47.718  51.945  1.00 20.08    A   O
ATOM   188 N   ASP A 26     26.174  47.562  54.044  1.00 19.15    A   N
ATOM   189 CA  ASP A 26     25.049  46.793  54.569  1.00 19.40    A   C
ATOM   190 CB  ASP A 26     25.524  45.978  55.768  1.00 21.39    A   C
ATOM   191 CG  ASP A 26     26.764  45.166  55.455  1.00 23.64    A   C
ATOM   192 OD1 ASP A 26     26.632  44.118  54.794  1.00 23.32    A   O
ATOM   193 OD2 ASP A 26     27.875  45.587  55.852  1.00 28.55    A   O
ATOM   194 C   ASP A 26     23.864  47.662  54.978  1.00 18.82    A   C
ATOM   195 O   ASP A 26     22.727  47.196  55.034  1.00 19.35    A   O
ATOM   196 N   GLU A 27     24.132  48.926  55.273  1.00 17.90    A   N
ATOM   197 CA  GLU A 27     23.067  49.840  55.671  1.00 17.07    A   C
ATOM   198 CB  GLU A 27     22.892  49.826  57.187  1.00 17.71    A   C
ATOM   199 CG  GLU A 27     21.646  50.550  57.663  1.00 24.75    A   C
ATOM   200 CD  GLU A 27     21.322  50.279  59.127  1.00 28.18    A   C
ATOM   201 OE1 GLU A 27     20.326  50.846  59.620  1.00 31.23    A   O
ATOM   202 OE2 GLU A 27     22.054  49.500  59.782  1.00 27.47    A   O
ATOM   203 C   GLU A 27     23.393  51.246  55.197  1.00 16.15    A   C
ATOM   204 O   GLU A 27     24.524  51.723  55.346  1.00 14.85    A   O
ATOM   205 N   ILE A 28     22.393  51.910  54.633  1.00 14.40    A   N
ATOM   206 CA  ILE A 28     22.577  53.257  54.118  1.00 12.75    A   C
ATOM   207 CB  ILE A 28     22.574  53.257  52.582  1.00 13.36    A   C
ATOM   208 CG2 ILE A 28     22.678  54.689  52.056  1.00  9.46    A   C
ATOM   209 CG1 ILE A 28     23.736  52.409  52.059  1.00 12.29    A   C
ATOM   210 CD1 ILE A 28     23.699  52.211  50.552  1.00 16.70    A   C
ATOM   211 C   ILE A 28     21.477  54.193  54.592  1.00 13.60    A   C
ATOM   212 O   ILE A 28     20.296  53.854  54.545  1.00 13.62    A   O
ATOM   213 N   ILE A 29     21.879  55.367  55.059  1.00 12.74    A   N
ATOM   214 CA  ILE A 29     20.928  56.375  55.507  1.00 14.14    A   C
ATOM   215 CB  ILE A 29     21.293  56.944  56.893  1.00 13.73    A   C
ATOM   216 CG2 ILE A 29     20.241  57.957  57.324  1.00 15.30    A   C
ATOM   217 CG1 ILE A 29     21.398  55.814  57.929  1.00 15.05    A   C
ATOM   218 CD1 ILE A 29     20.107  55.035  58.145  1.00 14.22    A   C
ATOM   219 C   ILE A 29     21.039  57.489  54.472  1.00 14.66    A   C
ATOM   220 O   ILE A 29     22.056  58.183  54.404  1.00 13.06    A   O
ATOM   221 N   TYR A 30     20.007  57.629  53.648  1.00 12.88    A   N
ATOM   222 CA  TYR A 30     19.987  58.649  52.609  1.00 14.23    A   C
ATOM   223 CB  TYR A 30     19.221  58.133  51.389  1.00 12.46    A   C
ATOM   224 CG  TYR A 30     19.221  59.075  50.205  1.00 15.02    A   C
ATOM   225 CD1 TYR A 30     20.155  58.933  49.178  1.00 12.86    A   C
ATOM   226 CE1 TYR A 30     20.171  59.803  48.088  1.00 12.85    A   C
ATOM   227 CD2 TYR A 30     18.298  60.119  50.117  1.00 15.96    A   C
ATOM   228 CE2 TYR A 30     18.304  60.996  49.034  1.00 15.05    A   C
ATOM   229 CZ  TYR A 30     19.243  60.831  48.023  1.00 14.12    A   C
ATOM   230 OH  TYR A 30     19.248  61.681  46.948  1.00 11.65    A   O
ATOM   231 C   TYR A 30     19.293  59.902  53.139  1.00 15.46    A   C
ATOM   232 O   TYR A 30     18.211  59.815  53.725  1.00 14.07    A   O
ATOM   233 N   TYR A 31     19.909  61.062  52.934  1.00 14.03    A   N
ATOM   234 CA  TYR A 31     19.297  62.312  53.370  1.00 14.37    A   C
ATOM   235 CB  TYR A 31     20.007  62.882  54.601  1.00 13.42    A   C
ATOM   236 CG  TYR A 31     19.441  64.216  55.045  1.00 13.73    A   C
ATOM   237 CD1 TYR A 31     18.150  64.307  55.559  1.00 15.42    A   C
ATOM   238 CE1 TYR A 31     17.616  65.532  55.962  1.00 18.80    A   C
ATOM   239 CD2 TYR A 31     20.191  65.389  54.940  1.00 15.22    A   C
ATOM   240 CE2 TYR A 31     19.665  66.625  55.335  1.00 19.27    A   C
ATOM   241 CZ  TYR A 31     18.376  66.686  55.847  1.00 20.56    A   C
ATOM   242 OH  TYR A 31     17.840  67.894  56.250  1.00 21.50    A   O
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Figure 6F

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ATOM   243  C   TYR A  31      19.321  63.355  52.257  1.00 13.94      A   C
ATOM   244  O   TYR A  31      20.383  63.704  51.743  1.00 12.53      A   O
ATOM   245  N   GLY A  32      18.139  63.836  51.876  1.00 14.52      A   N
ATOM   246  CA  GLY A  32      18.052  64.855  50.846  1.00 11.09      A   C
ATOM   247  C   GLY A  32      17.502  66.137  51.445  1.00 14.21      A   C
ATOM   248  O   GLY A  32      16.474  66.105  52.120  1.00 13.16      A   O
ATOM   249  N   ASP A  33      18.178  67.261  51.217  1.00 11.82      A   N
ATOM   250  CA  ASP A  33      17.728  68.550  51.754  1.00 12.90      A   C
ATOM   251  CB  ASP A  33      18.934  69.474  51.926  1.00 11.25      A   C
ATOM   252  CG  ASP A  33      18.576  70.788  52.587  1.00 11.81      A   C
ATOM   253  OD1 ASP A  33      17.562  70.842  53.309  1.00 14.26      A   O
ATOM   254  OD2 ASP A  33      19.326  71.757  52.394  1.00 11.68      A   O
ATOM   255  C   ASP A  33      16.703  69.145  50.783  1.00 13.65      A   C
ATOM   256  O   ASP A  33      16.824  70.285  50.324  1.00 12.95      A   O
ATOM   257  N   SER A  34      15.693  68.333  50.486  1.00 13.72      A   N
ATOM   258  CA  SER A  34      14.630  68.658  49.543  1.00 14.78      A   C
ATOM   259  CB  SER A  34      13.602  67.527  49.539  1.00 13.92      A   C
ATOM   260  OG  SER A  34      14.230  66.294  49.232  1.00 21.22      A   O
ATOM   261  C   SER A  34      13.914  69.980  49.751  1.00 16.62      A   C
ATOM   262  O   SER A  34      13.379  70.554  48.799  1.00 14.31      A   O
ATOM   263  N   ALA A  35      13.889  70.461  50.990  1.00 13.83      A   N
ATOM   264  CA  ALA A  35      13.216  71.717  51.282  1.00 14.72      A   C
ATOM   265  CB  ALA A  35      13.037  71.875  52.790  1.00 12.61      A   C
ATOM   266  C   ALA A  35      13.982  72.908  50.717  1.00 15.06      A   C
ATOM   267  O   ALA A  35      13.417  73.989  50.538  1.00 17.76      A   O
ATOM   268  N   ARG A  36      15.262  72.713  50.420  1.00 15.20      A   N
ATOM   269  CA  ARG A  36      16.076  73.804  49.902  1.00 15.09      A   C
ATOM   270  CB  ARG A  36      17.175  74.128  50.918  1.00 14.65      A   C
ATOM   271  CG  ARG A  36      16.585  74.462  52.284  1.00 13.95      A   C
ATOM   272  CD  ARG A  36      17.602  75.018  53.255  1.00 15.98      A   C
ATOM   273  NE  ARG A  36      18.579  74.020  53.681  1.00 14.55      A   N
ATOM   274  CZ  ARG A  36      19.333  74.141  54.769  1.00 19.35      A   C
ATOM   275  NH1 ARG A  36      19.217  75.221  55.537  1.00 16.64      A   N
ATOM   276  NH2 ARG A  36      20.201  73.187  55.093  1.00 16.02      A   N
ATOM   277  C   ARG A  36      16.668  73.578  48.511  1.00 15.81      A   C
ATOM   278  O   ARG A  36      17.422  74.409  48.002  1.00 15.67      A   O
ATOM   279  N   VAL A  37      16.319  72.461  47.888  1.00 15.48      A   N
ATOM   280  CA  VAL A  37      16.821  72.168  46.552  1.00 13.76      A   C
ATOM   281  CB  VAL A  37      16.374  70.746  46.115  1.00 14.93      A   C
ATOM   282  CG1 VAL A  37      14.877  70.727  45.851  1.00 14.99      A   C
ATOM   283  CG2 VAL A  37      17.174  70.280  44.898  1.00 14.00      A   C
ATOM   284  C   VAL A  37      16.246  73.243  45.617  1.00 11.66      A   C
ATOM   285  O   VAL A  37      15.112  73.697  45.805  1.00 11.22      A   O
ATOM   286  N   PRO A  38      17.011  73.662  44.596  1.00 12.05      A   N
ATOM   287  CD  PRO A  38      16.485  74.565  43.553  1.00 12.17      A   C
ATOM   288  CA  PRO A  38      18.356  73.214  44.244  1.00 13.67      A   C
ATOM   289  CB  PRO A  38      18.368  73.384  42.736  1.00 14.66      A   C
ATOM   290  CG  PRO A  38      17.655  74.698  42.588  1.00 12.08      A   C
ATOM   291  C   PRO A  38      19.486  74.000  44.898  1.00 15.15      A   C
ATOM   292  O   PRO A  38      19.297  75.129  45.370  1.00 12.96      A   O
ATOM   293  N   TYR A  39      20.664  73.382  44.900  1.00 11.07      A   N
ATOM   294  CA  TYR A  39      21.885  73.974  45.442  1.00 13.74      A   C
ATOM   295  CB  TYR A  39      22.796  72.893  46.040  1.00 11.65      A   C
ATOM   296  CG  TYR A  39      22.461  72.394  47.428  1.00 12.17      A   C
ATOM   297  CD1 TYR A  39      21.229  72.663  48.031  1.00 13.42      A   C
ATOM   298  CE1 TYR A  39      20.932  72.177  49.312  1.00 12.82      A   C
ATOM   299  CD2 TYR A  39      23.387  71.625  48.137  1.00 14.92      A   C
ATOM   300  CE2 TYR A  39      23.103  71.137  49.406  1.00 15.33      A   C
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Figure 6G

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ATOM   301  CZ  TYR A  39      21.878  71.414  49.992  1.00 13.34      A   C
ATOM   302  OH  TYR A  39      21.624  70.941  51.260  1.00 13.24      A   O
ATOM   303  C   TYR A  39      22.654  74.640  44.300  1.00 11.74      A   C
ATOM   304  O   TYR A  39      23.323  75.652  44.494  1.00 14.92      A   O
ATOM   305  N   GLY A  40      22.551  74.049  43.112  1.00 14.63      A   N
ATOM   306  CA  GLY A  40      23.269  74.529  41.939  1.00 12.47      A   C
ATOM   307  C   GLY A  40      23.196  75.993  41.544  1.00 14.09      A   C
ATOM   308  O   GLY A  40      24.093  76.502  40.871  1.00 12.63      A   O
ATOM   309  N   THR A  41      22.141  76.683  41.952  1.00 13.06      A   N
ATOM   310  CA  THR A  41      22.001  78.086  41.585  1.00 17.35      A   C
ATOM   311  CB  THR A  41      20.552  78.400  41.219  1.00 18.12      A   C
ATOM   312  OG1 THR A  41      19.713  78.078  42.332  1.00 22.00      A   O
ATOM   313  CG2 THR A  41      20.115  77.580  40.009  1.00 22.83      A   C
ATOM   314  C   THR A  41      22.416  79.020  42.712  1.00 16.33      A   C
ATOM   315  O   THR A  41      22.266  80.240  42.600  1.00 17.71      A   O
ATOM   316  N   LYS A  42      22.953  78.460  43.787  1.00 14.75      A   N
ATOM   317  CA  LYS A  42      23.331  79.281  44.922  1.00 13.75      A   C
ATOM   318  CB  LYS A  42      22.653  78.721  46.174  1.00 14.86      A   C
ATOM   319  CG  LYS A  42      21.139  78.899  46.078  1.00 14.53      A   C
ATOM   320  CD  LYS A  42      20.342  77.857  46.842  1.00 14.88      A   C
ATOM   321  CE  LYS A  42      18.898  77.878  46.349  1.00 13.95      A   C
ATOM   322  NZ  LYS A  42      17.995  76.929  47.073  1.00 12.60      A   N
ATOM   323  C   LYS A  42      24.824  79.496  45.119  1.00 16.57      A   C
ATOM   324  O   LYS A  42      25.647  78.943  44.391  1.00 14.82      A   O
ATOM   325  N   ASP A  43      25.157  80.329  46.099  1.00 17.21      A   N
ATOM   326  CA  ASP A  43      26.539  80.689  46.390  1.00 19.06      A   C
ATOM   327  CB  ASP A  43      26.567  82.117  46.932  1.00 20.48      A   C
ATOM   328  CG  ASP A  43      25.808  82.245  48.228  1.00 21.34      A   C
ATOM   329  OD1 ASP A  43      26.458  82.356  49.287  1.00 19.30      A   O
ATOM   330  OD2 ASP A  43      24.557  82.210  48.190  1.00 23.52      A   O
ATOM   331  C   ASP A  43      27.260  79.763  47.371  1.00 19.43      A   C
ATOM   332  O   ASP A  43      26.634  79.034  48.141  1.00 18.30      A   O
ATOM   333  N   PRO A  44      28.604  79.789  47.346  1.00 21.23      A   N
ATOM   334  CD  PRO A  44      29.401  80.567  46.377  1.00 20.65      A   C
ATOM   335  CA  PRO A  44      29.482  78.984  48.202  1.00 20.54      A   C
ATOM   336  CB  PRO A  44      30.866  79.543  47.886  1.00 20.91      A   C
ATOM   337  CG  PRO A  44      30.749  79.881  46.440  1.00 20.03      A   C
ATOM   338  C   PRO A  44      29.165  79.051  49.691  1.00 21.08      A   C
ATOM   339  O   PRO A  44      29.078  78.020  50.362  1.00 22.03      A   O
ATOM   340  N   THR A  45      28.999  80.266  50.207  1.00 20.06      A   N
ATOM   341  CA  THR A  45      28.707  80.453  51.622  1.00 19.83      A   C
ATOM   342  CB  THR A  45      28.523  81.953  51.961  1.00 22.19      A   C
ATOM   343  OG1 THR A  45      29.734  82.659  51.667  1.00 22.93      A   O
ATOM   344  CG2 THR A  45      28.180  82.135  53.429  1.00 21.29      A   C
ATOM   345  C   THR A  45      27.453  79.697  52.027  1.00 18.90      A   C
ATOM   346  O   THR A  45      27.448  78.950  53.007  1.00 16.82      A   O
ATOM   347  N   THR A  46      26.386  79.893  51.263  1.00 17.42      A   N
ATOM   348  CA  THR A  46      25.125  79.235  51.546  1.00 17.81      A   C
ATOM   349  CB  THR A  46      24.039  79.671  50.542  1.00 16.98      A   C
ATOM   350  OG1 THR A  46      23.835  81.087  50.636  1.00 17.53      A   O
ATOM   351  CG2 THR A  46      22.737  78.971  50.839  1.00 19.05      A   C
ATOM   352  C   THR A  46      25.265  77.719  51.484  1.00 17.51      A   C
ATOM   353  O   THR A  46      24.766  77.004  52.355  1.00 18.78      A   O
ATOM   354  N   ILE A  47      25.945  77.236  50.452  1.00 17.91      A   N
ATOM   355  CA  ILE A  47      26.134  75.803  50.265  1.00 20.81      A   C
ATOM   356  CB  ILE A  47      26.822  75.513  48.912  1.00 20.52      A   C
ATOM   357  CG2 ILE A  47      26.934  74.002  48.678  1.00 18.34      A   C
ATOM   358  CG1 ILE A  47      26.004  76.143  47.783  1.00 23.35      A   C
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Figure 6H

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ATOM   359 CD1 ILE A 47     24.523  75.792  47.826  1.00 23.82    A   C
ATOM   360 C   ILE A 47     26.935  75.170  51.398  1.00 19.27    A   C
ATOM   361 O   ILE A 47     26.568  74.111  51.905  1.00 21.96    A   O
ATOM   362 N   LYS A 48     28.018  75.818  51.805  1.00 21.30    A   N
ATOM   363 CA  LYS A 48     28.834  75.292  52.890  1.00 20.85    A   C
ATOM   364 CB  LYS A 48     30.032  76.203  53.151  1.00 22.83    A   C
ATOM   365 CG  LYS A 48     31.094  76.059  52.091  1.00 27.64    A   C
ATOM   366 CD  LYS A 48     32.380  76.794  52.444  1.00 31.38    A   C
ATOM   367 CE  LYS A 48     32.246  78.287  52.245  1.00 32.58    A   C
ATOM   368 NZ  LYS A 48     33.567  78.966  52.404  1.00 35.58    A   N
ATOM   369 C   LYS A 48     28.029  75.101  54.163  1.00 21.38    A   C
ATOM   370 O   LYS A 48     28.141  74.061  54.814  1.00 20.76    A   O
ATOM   371 N   GLN A 49     27.211  76.091  54.520  1.00 19.20    A   N
ATOM   372 CA  GLN A 49     26.395  75.963  55.716  1.00 19.40    A   C
ATOM   373 CB  GLN A 49     25.619  77.256  56.005  1.00 19.30    A   C
ATOM   374 CG  GLN A 49     24.776  77.203  57.286  1.00 22.44    A   C
ATOM   375 CD  GLN A 49     25.581  76.812  58.525  1.00 20.73    A   C
ATOM   376 OE1 GLN A 49     26.740  77.192  58.667  1.00 22.79    A   O
ATOM   377 NE2 GLN A 49     24.958  76.068  59.433  1.00 22.60    A   N
ATOM   378 C   GLN A 49     25.423  74.803  55.553  1.00 18.14    A   C
ATOM   379 O   GLN A 49     25.159  74.074  56.510  1.00 19.87    A   O
ATOM   380 N   PHE A 50     24.882  74.631  54.348  1.00 17.65    A   N
ATOM   381 CA  PHE A 50     23.960  73.521  54.112  1.00 17.56    A   C
ATOM   382 CB  PHE A 50     23.461  73.510  52.659  1.00 17.20    A   C
ATOM   383 CG  PHE A 50     22.478  74.604  52.331  1.00 18.53    A   C
ATOM   384 CD1 PHE A 50     21.961  75.433  53.323  1.00 18.95    A   C
ATOM   385 CD2 PHE A 50     22.041  74.780  51.022  1.00 20.21    A   C
ATOM   386 CE1 PHE A 50     21.023  76.418  53.022  1.00 19.32    A   C
ATOM   387 CE2 PHE A 50     21.101  75.763  50.709  1.00 22.48    A   C
ATOM   388 CZ  PHE A 50     20.592  76.583  51.716  1.00 21.15    A   C
ATOM   389 C   PHE A 50     24.706  72.217  54.401  1.00 15.70    A   C
ATOM   390 O   PHE A 50     24.178  71.311  55.048  1.00 15.38    A   O
ATOM   391 N   GLY A 51     25.945  72.143  53.922  1.00 18.19    A   N
ATOM   392 CA  GLY A 51     26.760  70.959  54.126  1.00 19.41    A   C
ATOM   393 C   GLY A 51     27.006  70.667  55.592  1.00 20.96    A   C
ATOM   394 O   GLY A 51     26.964  69.514  56.026  1.00 20.04    A   O
ATOM   395 N   LEU A 52     27.261  71.716  56.368  1.00 22.33    A   N
ATOM   396 CA  LEU A 52     27.508  71.542  57.791  1.00 22.23    A   C
ATOM   397 CB  LEU A 52     27.995  72.855  58.412  1.00 24.46    A   C
ATOM   398 CG  LEU A 52     29.385  73.328  57.980  1.00 25.92    A   C
ATOM   399 CD1 LEU A 52     29.734  74.618  58.719  1.00 28.98    A   C
ATOM   400 CD2 LEU A 52     30.423  72.249  58.293  1.00 27.40    A   C
ATOM   401 C   LEU A 52     26.246  71.063  58.493  1.00 21.84    A   C
ATOM   402 O   LEU A 52     26.294  70.180  59.344  1.00 21.12    A   O
ATOM   403 N   GLU A 53     25.107  71.635  58.124  1.00 20.72    A   N
ATOM   404 CA  GLU A 53     23.852  71.237  58.736  1.00 20.40    A   C
ATOM   405 CB  GLU A 53     22.731  72.185  58.294  1.00 21.74    A   C
ATOM   406 CG  GLU A 53     22.655  73.438  59.159  1.00 21.95    A   C
ATOM   407 CD  GLU A 53     21.839  74.551  58.536  1.00 23.86    A   C
ATOM   408 OE1 GLU A 53     20.797  74.260  57.906  1.00 23.19    A   O
ATOM   409 OE2 GLU A 53     22.238  75.727  58.685  1.00 24.44    A   O
ATOM   410 C   GLU A 53     23.514  69.789  58.405  1.00 19.46    A   C
ATOM   411 O   GLU A 53     22.813  69.122  59.160  1.00 22.12    A   O
ATOM   412 N   ALA A 54     24.022  69.295  57.282  1.00 20.85    A   N
ATOM   413 CA  ALA A 54     23.760  67.910  56.905  1.00 18.16    A   C
ATOM   414 CB  ALA A 54     24.252  67.647  55.498  1.00 16.88    A   C
ATOM   415 C   ALA A 54     24.474  66.997  57.899  1.00 18.85    A   C
ATOM   416 O   ALA A 54     23.953  65.944  58.280  1.00 18.10    A   O
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Figure 6I

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ATOM   417 N   LEU A 55     25.670 67.408 58.313 1.00 19.45    A   N
ATOM   418 CA  LEU A 55     26.442 66.639 59.281 1.00 19.66    A   C
ATOM   419 CB  LEU A 55     27.775 67.329 59.590 1.00 21.26    A   C
ATOM   420 CG  LEU A 55     28.782 67.408 58.442 1.00 22.31    A   C
ATOM   421 CD1 LEU A 55     30.070 68.042 58.935 1.00 21.17    A   C
ATOM   422 CD2 LEU A 55     29.055 66.008 57.898 1.00 22.77    A   C
ATOM   423 C   LEU A 55     25.626 66.504 60.556 1.00 21.84    A   C
ATOM   424 O   LEU A 55     25.589 65.437 61.166 1.00 20.58    A   O
ATOM   425 N   ASP A 56     24.959 67.584 60.953 1.00 21.85    A   N
ATOM   426 CA  ASP A 56     24.147 67.543 62.157 1.00 22.53    A   C
ATOM   427 CB  ASP A 56     23.506 68.904 62.437 1.00 25.87    A   C
ATOM   428 CG  ASP A 56     24.530 69.986 62.715 1.00 29.28    A   C
ATOM   429 OD1 ASP A 56     25.636 69.651 63.190 1.00 31.33    A   O
ATOM   430 OD2 ASP A 56     24.226 71.172 62.473 1.00 32.07    A   O
ATOM   431 C   ASP A 56     23.062 66.492 62.023 1.00 22.75    A   C
ATOM   432 O   ASP A 56     22.777 65.762 62.974 1.00 22.74    A   O
ATOM   433 N   PHE A 57     22.459 66.403 60.841 1.00 20.21    A   N
ATOM   434 CA  PHE A 57     21.404 65.422 60.633 1.00 21.09    A   C
ATOM   435 CB  PHE A 57     20.831 65.497 59.215 1.00 21.92    A   C
ATOM   436 CG  PHE A 57     19.915 64.352 58.893 1.00 21.43    A   C
ATOM   437 CD1 PHE A 57     18.609 64.336 59.370 1.00 22.87    A   C
ATOM   438 CD2 PHE A 57     20.393 63.233 58.214 1.00 20.64    A   C
ATOM   439 CE1 PHE A 57     17.792 63.218 59.184 1.00 20.01    A   C
ATOM   440 CE2 PHE A 57     19.589 62.112 58.024 1.00 21.14    A   C
ATOM   441 CZ  PHE A 57     18.286 62.104 58.512 1.00 23.52    A   C
ATOM   442 C   PHE A 57     21.873 63.991 60.864 1.00 18.61    A   C
ATOM   443 O   PHE A 57     21.148 63.181 61.441 1.00 20.52    A   O
ATOM   444 N   PHE A 58     23.081 63.679 60.408 1.00 19.51    A   N
ATOM   445 CA  PHE A 58     23.615 62.324 60.532 1.00 21.64    A   C
ATOM   446 CB  PHE A 58     24.701 62.097 59.478 1.00 18.15    A   C
ATOM   447 CG  PHE A 58     24.181 62.018 58.072 1.00 17.07    A   C
ATOM   448 CD1 PHE A 58     24.380 63.072 57.180 1.00 15.61    A   C
ATOM   449 CD2 PHE A 58     23.508 60.878 57.628 1.00 16.58    A   C
ATOM   450 CE1 PHE A 58     23.920 62.993 55.868 1.00 16.17    A   C
ATOM   451 CE2 PHE A 58     23.044 60.790 56.318 1.00 20.24    A   C
ATOM   452 CZ  PHE A 58     23.251 61.850 55.436 1.00 14.25    A   C
ATOM   453 C   PHE A 58     24.164 61.894 61.896 1.00 24.25    A   C
ATOM   454 O   PHE A 58     24.323 60.697 62.147 1.00 24.91    A   O
ATOM   455 N   LYS A 59     24.449 62.850 62.774 1.00 26.87    A   N
ATOM   456 CA  LYS A 59     25.014 62.528 64.087 1.00 28.83    A   C
ATOM   457 CB  LYS A 59     25.116 63.800 64.931 1.00 31.02    A   C
ATOM   458 CG  LYS A 59     26.127 64.792 64.374 1.00 33.56    A   C
ATOM   459 CD  LYS A 59     26.237 66.047 65.221 1.00 37.86    A   C
ATOM   460 CE  LYS A 59     27.270 67.000 64.632 1.00 38.94    A   C
ATOM   461 NZ  LYS A 59     27.433 68.240 65.443 1.00 41.75    A   N
ATOM   462 C   LYS A 59     24.312 61.419 64.879 1.00 28.21    A   C
ATOM   463 O   LYS A 59     24.973 60.541 65.439 1.00 28.12    A   O
ATOM   464 N   PRO A 60     22.969 61.437 64.933 1.00 27.85    A   N
ATOM   465 CD  PRO A 60     22.061 62.472 64.412 1.00 27.44    A   C
ATOM   466 CA  PRO A 60     22.219 60.409 65.671 1.00 26.21    A   C
ATOM   467 CB  PRO A 60     20.791 60.962 65.691 1.00 28.29    A   C
ATOM   468 CG  PRO A 60     20.961 62.446 65.419 1.00 29.74    A   C
ATOM   469 C   PRO A 60     22.264 59.040 64.994 1.00 25.09    A   C
ATOM   470 O   PRO A 60     22.116 58.004 65.640 1.00 24.61    A   O
ATOM   471 N   HIS A 61     22.469 59.045 63.682 1.00 24.30    A   N
ATOM   472 CA  HIS A 61     22.489 57.815 62.906 1.00 23.28    A   C
ATOM   473 CB  HIS A 61     22.210 58.148 61.445 1.00 23.75    A   C
ATOM   474 CG  HIS A 61     20.813 58.616 61.202 1.00 23.81    A   C
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Figure 6J

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ATOM   475 CD2 HIS A 61     20.307  59.858  61.017  1.00 24.28    A   C
ATOM   476 ND1 HIS A 61     19.738  57.753  61.163  1.00 21.57    A   N
ATOM   477 CE1 HIS A 61     18.631  58.443  60.963  1.00 21.88    A   C
ATOM   478 NE2 HIS A 61     18.948  59.723  60.871  1.00 24.37    A   N
ATOM   479 C   HIS A 61     23.754  56.979  63.012  1.00 23.45    A   C
ATOM   480 O   HIS A 61     23.812  55.879  62.475  1.00 23.17    A   O
ATOM   481 N   GLU A 62     24.752  57.497  63.718  1.00 26.52    A   N
ATOM   482 CA  GLU A 62     26.030  56.811  63.892  1.00 27.77    A   C
ATOM   483 CB  GLU A 62     25.944  55.818  65.062  1.00 33.97    A   C
ATOM   484 CG  GLU A 62     24.861  54.754  64.943  1.00 37.16    A   C
ATOM   485 CD  GLU A 62     24.468  54.176  66.292  1.00 40.46    A   C
ATOM   486 OE1 GLU A 62     25.367  53.907  67.117  1.00 41.12    A   O
ATOM   487 OE2 GLU A 62     23.255  53.983  66.525  1.00 42.43    A   O
ATOM   488 C   GLU A 62     26.545  56.118  62.626  1.00 26.21    A   C
ATOM   489 O   GLU A 62     26.699  54.897  62.579  1.00 26.16    A   O
ATOM   490 N   ILE A 63     26.798  56.913  61.591  1.00 22.24    A   N
ATOM   491 CA  ILE A 63     27.333  56.385  60.338  1.00 21.10    A   C
ATOM   492 CB  ILE A 63     26.904  57.246  59.124  1.00 19.78    A   C
ATOM   493 CG2 ILE A 63     25.416  57.065  58.859  1.00 15.78    A   C
ATOM   494 CG1 ILE A 63     27.224  58.718  59.388  1.00 16.88    A   C
ATOM   495 CD1 ILE A 63     27.000  59.636  58.189  1.00 18.48    A   C
ATOM   496 C   ILE A 63     28.853  56.420  60.483  1.00 18.95    A   C
ATOM   497 O   ILE A 63     29.385  57.182  61.293  1.00 19.85    A   O
ATOM   498 N   GLU A 64     29.553  55.593  59.718  1.00 19.95    A   N
ATOM   499 CA  GLU A 64     31.008  55.561  59.804  1.00 19.49    A   C
ATOM   500 CB  GLU A 64     31.492  54.118  59.926  1.00 22.43    A   C
ATOM   501 CG  GLU A 64     31.139  53.498  61.268  1.00 26.80    A   C
ATOM   502 CD  GLU A 64     31.762  52.136  61.452  1.00 29.61    A   C
ATOM   503 OE1 GLU A 64     33.012  52.044  61.421  1.00 31.41    A   O
ATOM   504 OE2 GLU A 64     31.003  51.160  61.623  1.00 29.53    A   O
ATOM   505 C   GLU A 64     31.684  56.251  58.630  1.00 17.37    A   C
ATOM   506 O   GLU A 64     32.890  56.453  58.631  1.00 16.28    A   O
ATOM   507 N   LEU A 65     30.890  56.615  57.632  1.00 18.28    A   N
ATOM   508 CA  LEU A 65     31.393  57.308  56.456  1.00 17.15    A   C
ATOM   509 CB  LEU A 65     32.035  56.318  55.478  1.00 18.66    A   C
ATOM   510 CG  LEU A 65     32.582  56.903  54.169  1.00 21.47    A   C
ATOM   511 CD1 LEU A 65     33.667  55.991  53.603  1.00 23.00    A   C
ATOM   512 CD2 LEU A 65     31.449  57.086  53.167  1.00 22.69    A   C
ATOM   513 C   LEU A 65     30.230  58.021  55.786  1.00 16.52    A   C
ATOM   514 O   LEU A 65     29.100  57.539  55.813  1.00 14.91    A   O
ATOM   515 N   LEU A 66     30.510  59.180  55.204  1.00 14.90    A   N
ATOM   516 CA  LEU A 66     29.486  59.946  54.526  1.00 14.23    A   C
ATOM   517 CB  LEU A 66     29.264  61.288  55.231  1.00 14.12    A   C
ATOM   518 CG  LEU A 66     28.297  62.240  54.514  1.00 14.20    A   C
ATOM   519 CD1 LEU A 66     26.932  61.586  54.415  1.00 14.73    A   C
ATOM   520 CD2 LEU A 66     28.195  63.562  55.262  1.00 13.86    A   C
ATOM   521 C   LEU A 66     29.864  60.200  53.077  1.00 14.92    A   C
ATOM   522 O   LEU A 66     30.975  60.642  52.773  1.00 14.96    A   O
ATOM   523 N   ILE A 67     28.938  59.886  52.181  1.00 13.46    A   N
ATOM   524 CA  ILE A 67     29.140  60.124  50.766  1.00 12.96    A   C
ATOM   525 CB  ILE A 67     28.641  58.953  49.886  1.00 13.86    A   C
ATOM   526 CG2 ILE A 67     28.617  59.385  48.419  1.00 12.97    A   C
ATOM   527 CG1 ILE A 67     29.541  57.729  50.066  1.00 14.37    A   C
ATOM   528 CD1 ILE A 67     29.105  56.530  49.237  1.00 18.27    A   C
ATOM   529 C   ILE A 67     28.314  61.346  50.406  1.00 12.36    A   C
ATOM   530 O   ILE A 67     27.116  61.420  50.719  1.00 13.82    A   O
ATOM   531 N   VAL A 68     28.964  62.317  49.780  1.00 12.37    A   N
ATOM   532 CA  VAL A 68     28.275  63.516  49.342  1.00 12.34    A   C
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Figure 6K

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ATOM   533 CB  VAL A 68    29.160  64.759  49.466  1.00 10.71    A   C
ATOM   534 CG1 VAL A 68    28.413  65.977  48.916  1.00 10.16    A   C
ATOM   535 CG2 VAL A 68    29.525  64.978  50.927  1.00 11.52    A   C
ATOM   536 C   VAL A 68    28.002  63.222  47.884  1.00 11.20    A   C
ATOM   537 O   VAL A 68    28.885  63.362  47.038  1.00 12.44    A   O
ATOM   538 N   ALA A 69    26.785  62.775  47.602  1.00  9.18    A   N
ATOM   539 CA  ALA A 69    26.405  62.415  46.244  1.00 10.89    A   C
ATOM   540 CB  ALA A 69    25.129  61.581  46.263  1.00  9.29    A   C
ATOM   541 C   ALA A 69    26.218  63.631  45.358  1.00 10.34    A   C
ATOM   542 O   ALA A 69    26.341  63.546  44.139  1.00 11.20    A   O
ATOM   543 N   CYS A 70    25.905  64.760  45.982  1.00 10.65    A   N
ATOM   544 CA  CYS A 70    25.692  66.000  45.253  1.00 11.99    A   C
ATOM   545 CB  CYS A 70    25.026  67.030  46.167  1.00 13.56    A   C
ATOM   546 SG  CYS A 70    24.697  68.605  45.370  1.00 10.79    A   S
ATOM   547 C   CYS A 70    27.004  66.560  44.720  1.00 11.25    A   C
ATOM   548 O   CYS A 70    27.981  66.708  45.463  1.00  9.23    A   O
ATOM   549 N   ASN A 71    27.030  66.867  43.425  1.00 10.81    A   N
ATOM   550 CA  ASN A 71    28.228  67.424  42.807  1.00  9.85    A   C
ATOM   551 CB  ASN A 71    28.120  67.369  41.285  1.00  7.25    A   C
ATOM   552 CG  ASN A 71    28.026  65.959  40.768  1.00  9.24    A   C
ATOM   553 OD1 ASN A 71    26.998  65.298  40.919  1.00  8.82    A   O
ATOM   554 ND2 ASN A 71    29.107  65.478  40.165  1.00  9.13    A   N
ATOM   555 C   ASN A 71    28.434  68.866  43.246  1.00 12.09    A   C
ATOM   556 O   ASN A 71    29.565  69.321  43.432  1.00  9.50    A   O
ATOM   557 N   THR A 72    27.337  69.593  43.399  1.00 10.94    A   N
ATOM   558 CA  THR A 72    27.436  70.975  43.834  1.00 10.39    A   C
ATOM   559 CB  THR A 72    26.073  71.676  43.779  1.00  9.07    A   C
ATOM   560 OG1 THR A 72    25.599  71.675  42.429  1.00 10.15    A   O
ATOM   561 CG2 THR A 72    26.200  73.122  44.262  1.00  9.53    A   C
ATOM   562 C   THR A 72    27.974  71.029  45.259  1.00 11.47    A   C
ATOM   563 O   THR A 72    28.882  71.808  45.556  1.00  9.49    A   O
ATOM   564 N   ALA A 73    27.415  70.202  46.144  1.00 13.67    A   N
ATOM   565 CA  ALA A 73    27.871  70.171  47.531  1.00 13.27    A   C
ATOM   566 CB  ALA A 73    26.979  69.251  48.368  1.00 15.12    A   C
ATOM   567 C   ALA A 73    29.318  69.691  47.586  1.00 15.74    A   C
ATOM   568 O   ALA A 73    30.111  70.160  48.412  1.00 15.99    A   O
ATOM   569 N   SER A 74    29.660  68.746  46.714  1.00 13.48    A   N
ATOM   570 CA  SER A 74    31.021  68.226  46.677  1.00 13.55    A   C
ATOM   571 CB  SER A 74    31.133  67.078  45.666  1.00 10.32    A   C
ATOM   572 OG  SER A 74    30.483  65.916  46.148  1.00 14.22    A   O
ATOM   573 C   SER A 74    31.994  69.333  46.297  1.00 15.60    A   C
ATOM   574 O   SER A 74    33.093  69.439  46.845  1.00 14.18    A   O
ATOM   575 N   ALA A 75    31.578  70.169  45.359  1.00 13.93    A   N
ATOM   576 CA  ALA A 75    32.422  71.259  44.899  1.00 15.79    A   C
ATOM   577 CB  ALA A 75    31.899  71.773  43.560  1.00 16.15    A   C
ATOM   578 C   ALA A 75    32.549  72.420  45.886  1.00 17.44    A   C
ATOM   579 O   ALA A 75    33.639  72.967  46.063  1.00 18.83    A   O
ATOM   580 N   LEU A 76    31.453  72.777  46.548  1.00 15.33    A   N
ATOM   581 CA  LEU A 76    31.462  73.920  47.460  1.00 17.71    A   C
ATOM   582 CB  LEU A 76    30.236  74.793  47.189  1.00 16.64    A   C
ATOM   583 CG  LEU A 76    30.154  75.642  45.917  1.00 19.98    A   C
ATOM   584 CD1 LEU A 76    30.338  74.793  44.681  1.00 15.78    A   C
ATOM   585 CD2 LEU A 76    28.801  76.343  45.886  1.00 19.48    A   C
ATOM   586 C   LEU A 76    31.544  73.693  48.967  1.00 18.84    A   C
ATOM   587 O   LEU A 76    32.101  74.531  49.685  1.00 17.49    A   O
ATOM   588 N   ALA A 77    30.996  72.584  49.456  1.00 16.91    A   N
ATOM   589 CA  ALA A 77    30.986  72.338  50.896  1.00 17.45    A   C
ATOM   590 CB  ALA A 77    29.546  72.118  51.363  1.00 15.97    A   C
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Figure 6L

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ATOM   591  C   ALA A  77      31.862  71.206  51.422  1.00 17.05      A   C
ATOM   592  O   ALA A  77      32.092  71.120  52.630  1.00 15.31      A   O
ATOM   593  N   LEU A  78      32.355  70.350  50.533  1.00 17.95      A   N
ATOM   594  CA  LEU A  78      33.173  69.217  50.950  1.00 18.28      A   C
ATOM   595  CB  LEU A  78      33.701  68.456  49.726  1.00 17.49      A   C
ATOM   596  CG  LEU A  78      34.425  67.141  50.053  1.00 18.47      A   C
ATOM   597  CD1 LEU A  78      33.467  66.196  50.771  1.00 13.07      A   C
ATOM   598  CD2 LEU A  78      34.949  66.493  48.772  1.00 15.57      A   C
ATOM   599  C   LEU A  78      34.337  69.572  51.873  1.00 19.44      A   C
ATOM   600  O   LEU A  78      34.478  68.986  52.944  1.00 17.85      A   O
ATOM   601  N   GLU A  79      35.173  70.524  51.472  1.00 20.74      A   N
ATOM   602  CA  GLU A  79      36.310  70.897  52.304  1.00 23.29      A   C
ATOM   603  CB  GLU A  79      37.112  72.023  51.652  1.00 25.50      A   C
ATOM   604  CG  GLU A  79      38.332  72.435  52.464  1.00 32.40      A   C
ATOM   605  CD  GLU A  79      39.248  73.382  51.714  1.00 36.37      A   C
ATOM   606  OE1 GLU A  79      38.811  74.501  51.377  1.00 38.33      A   O
ATOM   607  OE2 GLU A  79      40.411  73.002  51.459  1.00 40.30      A   O
ATOM   608  C   GLU A  79      35.900  71.312  53.716  1.00 22.08      A   C
ATOM   609  O   GLU A  79      36.512  70.888  54.691  1.00 22.83      A   O
ATOM   610  N   GLU A  80      34.862  72.132  53.825  1.00 22.05      A   N
ATOM   611  CA  GLU A  80      34.399  72.591  55.125  1.00 21.68      A   C
ATOM   612  CB  GLU A  80      33.336  73.675  54.957  1.00 26.13      A   C
ATOM   613  CG  GLU A  80      33.081  74.457  56.232  1.00 32.22      A   C
ATOM   614  CD  GLU A  80      34.173  75.479  56.521  1.00 34.38      A   C
ATOM   615  OE1 GLU A  80      35.371  75.145  56.399  1.00 36.64      A   O
ATOM   616  OE2 GLU A  80      33.828  76.623  56.878  1.00 38.94      A   O
ATOM   617  C   GLU A  80      33.823  71.435  55.939  1.00 21.19      A   C
ATOM   618  O   GLU A  80      34.013  71.359  57.152  1.00 20.49      A   O
ATOM   619  N   MET A  81      33.116  70.533  55.269  1.00 18.90      A   N
ATOM   620  CA  MET A  81      32.531  69.389  55.950  1.00 16.84      A   C
ATOM   621  CB  MET A  81      31.639  68.605  54.992  1.00 14.00      A   C
ATOM   622  CG  MET A  81      30.375  69.349  54.615  1.00 15.86      A   C
ATOM   623  SD  MET A  81      29.517  68.583  53.244  1.00 15.74      A   S
ATOM   624  CE  MET A  81      28.866  67.134  54.019  1.00 14.04      A   C
ATOM   625  C   MET A  81      33.618  68.474  56.503  1.00 17.31      A   C
ATOM   626  O   MET A  81      33.539  68.020  57.646  1.00 16.49      A   O
ATOM   627  N   GLN A  82      34.632  68.216  55.684  1.00 18.90      A   N
ATOM   628  CA  GLN A  82      35.739  67.351  56.078  1.00 22.12      A   C
ATOM   629  CB  GLN A  82      36.674  67.125  54.887  1.00 22.92      A   C
ATOM   630  CG  GLN A  82      36.001  66.442  53.706  1.00 21.03      A   C
ATOM   631  CD  GLN A  82      36.961  66.158  52.575  1.00 22.15      A   C
ATOM   632  OE1 GLN A  82      37.725  67.033  52.159  1.00 22.13      A   O
ATOM   633  NE2 GLN A  82      36.924  64.934  52.061  1.00 20.69      A   N
ATOM   634  C   GLN A  82      36.516  67.956  57.237  1.00 24.53      A   C
ATOM   635  O   GLN A  82      37.051  67.239  58.086  1.00 23.68      A   O
ATOM   636  N   LYS A  83      36.565  69.282  57.271  1.00 26.24      A   N
ATOM   637  CA  LYS A  83      37.282  69.993  58.317  1.00 30.03      A   C
ATOM   638  CB  LYS A  83      37.178  71.505  58.092  1.00 30.40      A   C
ATOM   639  CG  LYS A  83      38.023  72.336  59.041  1.00 34.26      A   C
ATOM   640  CD  LYS A  83      37.873  73.829  58.756  1.00 38.51      A   C
ATOM   641  CE  LYS A  83      38.287  74.175  57.329  1.00 42.25      A   C
ATOM   642  NZ  LYS A  83      38.067  75.619  57.005  1.00 43.57      A   N
ATOM   643  C   LYS A  83      36.764  69.650  59.708  1.00 30.42      A   C
ATOM   644  O   LYS A  83      37.551  69.395  60.616  1.00 31.77      A   O
ATOM   645  N   TYR A  84      35.445  69.624  59.870  1.00 30.72      A   N
ATOM   646  CA  TYR A  84      34.850  69.341  61.173  1.00 34.49      A   C
ATOM   647  CB  TYR A  84      33.702  70.322  61.441  1.00 38.58      A   C
ATOM   648  CG  TYR A  84      34.109  71.781  61.386  1.00 43.85      A   C
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Figure 6M

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ATOM   649 CD1 TYR A 84     34.172  72.465  60.169  1.00 45.26    A   C
ATOM   650 CE1 TYR A 84     34.575  73.803  60.111  1.00 46.74    A   C
ATOM   651 CD2 TYR A 84     34.460  72.472  62.549  1.00 45.80    A   C
ATOM   652 CE2 TYR A 84     34.865  73.808  62.501  1.00 47.25    A   C
ATOM   653 CZ  TYR A 84     34.920  74.467  61.281  1.00 47.45    A   C
ATOM   654 OH  TYR A 84     35.321  75.784  61.233  1.00 47.13    A   O
ATOM   655 C   TYR A 84     34.349  67.911  61.401  1.00 33.43    A   C
ATOM   656 O   TYR A 84     33.973  67.555  62.520  1.00 34.46    A   O
ATOM   657 N   SER A 85     34.348  67.088  60.361  1.00 30.46    A   N
ATOM   658 CA  SER A 85     33.865  65.721  60.507  1.00 27.21    A   C
ATOM   659 CB  SER A 85     33.384  65.192  59.160  1.00 26.99    A   C
ATOM   660 OG  SER A 85     33.003  63.836  59.279  1.00 27.59    A   O
ATOM   661 C   SER A 85     34.883  64.745  61.088  1.00 25.50    A   C
ATOM   662 O   SER A 85     36.059  64.778  60.730  1.00 24.71    A   O
ATOM   663 N   LYS A 86     34.415  63.875  61.981  1.00 23.68    A   N
ATOM   664 CA  LYS A 86     35.265  62.868  62.609  1.00 23.93    A   C
ATOM   665 CB  LYS A 86     34.741  62.509  64.005  1.00 26.65    A   C
ATOM   666 CG  LYS A 86     34.774  63.644  65.028  1.00 31.69    A   C
ATOM   667 CD  LYS A 86     36.190  63.990  65.491  1.00 34.31    A   C
ATOM   668 CE  LYS A 86     37.015  64.657  64.401  1.00 35.72    A   C
ATOM   669 NZ  LYS A 86     38.359  65.087  64.902  1.00 41.28    A   N
ATOM   670 C   LYS A 86     35.308  61.607  61.752  1.00 22.61    A   C
ATOM   671 O   LYS A 86     36.192  60.765  61.914  1.00 23.21    A   O
ATOM   672 N   ILE A 87     34.337  61.462  60.857  1.00 19.67    A   N
ATOM   673 CA  ILE A 87     34.305  60.302  59.975  1.00 18.68    A   C
ATOM   674 CB  ILE A 87     32.896  59.681  59.888  1.00 18.75    A   C
ATOM   675 CG2 ILE A 87     32.510  59.090  61.233  1.00 18.89    A   C
ATOM   676 CG1 ILE A 87     31.887  60.742  59.433  1.00 21.06    A   C
ATOM   677 CD1 ILE A 87     30.508  60.187  59.086  1.00 18.90    A   C
ATOM   678 C   ILE A 87     34.720  60.751  58.585  1.00 16.98    A   C
ATOM   679 O   ILE A 87     34.614  61.932  58.248  1.00 16.62    A   O
ATOM   680 N   PRO A 88     35.219  59.822  57.761  1.00 17.72    A   N
ATOM   681 CD  PRO A 88     35.548  58.403  57.992  1.00 17.09    A   C
ATOM   682 CA  PRO A 88     35.616  60.247  56.418  1.00 17.99    A   C
ATOM   683 CB  PRO A 88     36.319  59.011  55.857  1.00 19.59    A   C
ATOM   684 CG  PRO A 88     35.648  57.872  56.587  1.00 18.28    A   C
ATOM   685 C   PRO A 88     34.411  60.672  55.577  1.00 19.00    A   C
ATOM   686 O   PRO A 88     33.318  60.125  55.711  1.00 17.80    A   O
ATOM   687 N   ILE A 89     34.622  61.668  54.726  1.00 19.35    A   N
ATOM   688 CA  ILE A 89     33.577  62.163  53.843  1.00 18.35    A   C
ATOM   689 CB  ILE A 89     33.171  63.613  54.196  1.00 18.03    A   C
ATOM   690 CG2 ILE A 89     32.157  64.136  53.185  1.00 16.99    A   C
ATOM   691 CG1 ILE A 89     32.562  63.641  55.598  1.00 18.30    A   C
ATOM   692 CD1 ILE A 89     32.020  64.990  56.011  1.00 26.25    A   C
ATOM   693 C   ILE A 89     34.134  62.108  52.429  1.00 17.01    A   C
ATOM   694 O   ILE A 89     35.206  62.646  52.144  1.00 18.36    A   O
ATOM   695 N   VAL A 90     33.406  61.435  51.551  1.00 15.45    A   N
ATOM   696 CA  VAL A 90     33.829  61.270  50.173  1.00 14.79    A   C
ATOM   697 CB  VAL A 90     33.899  59.779  49.806  1.00 14.33    A   C
ATOM   698 CG1 VAL A 90     34.409  59.605  48.389  1.00 12.10    A   C
ATOM   699 CG2 VAL A 90     34.804  59.055  50.796  1.00 15.51    A   C
ATOM   700 C   VAL A 90     32.858  61.957  49.234  1.00 14.94    A   C
ATOM   701 O   VAL A 90     31.658  61.702  49.283  1.00 15.20    A   O
ATOM   702 N   GLY A 91     33.391  62.830  48.387  1.00 13.93    A   N
ATOM   703 CA  GLY A 91     32.570  63.540  47.427  1.00 14.67    A   C
ATOM   704 C   GLY A 91     32.606  62.829  46.087  1.00 15.17    A   C
ATOM   705 O   GLY A 91     33.262  61.794  45.937  1.00 15.39    A   O
ATOM   706 N   VAL A 92     31.921  63.391  45.101  1.00 13.28    A   N
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Figure 6N

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ATOM   707 CA  VAL A  92     31.871  62.777  43.782  1.00 15.09    A   C
ATOM   708 CB  VAL A  92     30.434  62.762  43.243  1.00 14.78    A   C
ATOM   709 CG1 VAL A  92     29.629  61.703  43.977  1.00 14.03    A   C
ATOM   710 CG2 VAL A  92     29.793  64.135  43.412  1.00 10.70    A   C
ATOM   711 C   VAL A  92     32.770  63.405  42.730  1.00 14.63    A   C
ATOM   712 O   VAL A  92     32.739  63.006  41.567  1.00 17.71    A   O
ATOM   713 N   ILE A  93     33.578  64.378  43.128  1.00 15.55    A   N
ATOM   714 CA  ILE A  93     34.468  65.025  42.176  1.00 16.08    A   C
ATOM   715 CB  ILE A  93     34.684  66.497  42.561  1.00 16.56    A   C
ATOM   716 CG2 ILE A  93     35.653  67.169  41.589  1.00 11.15    A   C
ATOM   717 CG1 ILE A  93     33.329  67.210  42.555  1.00 17.56    A   C
ATOM   718 CD1 ILE A  93     33.385  68.627  43.056  1.00 24.35    A   C
ATOM   719 C   ILE A  93     35.812  64.304  42.032  1.00 15.47    A   C
ATOM   720 O   ILE A  93     36.180  63.904  40.926  1.00 14.93    A   O
ATOM   721 N   GLU A  94     36.536  64.118  43.132  1.00 16.92    A   N
ATOM   722 CA  GLU A  94     37.831  63.446  43.052  1.00 16.92    A   C
ATOM   723 CB  GLU A  94     38.471  63.305  44.434  1.00 20.92    A   C
ATOM   724 CG  GLU A  94     39.894  62.754  44.361  1.00 26.29    A   C
ATOM   725 CD  GLU A  94     40.576  62.678  45.713  1.00 32.62    A   C
ATOM   726 OE1 GLU A  94     40.310  61.723  46.474  1.00 35.02    A   O
ATOM   727 OE2 GLU A  94     41.377  63.588  46.019  1.00 37.91    A   O
ATOM   728 C   GLU A  94     37.745  62.067  42.399  1.00 16.23    A   C
ATOM   729 O   GLU A  94     38.594  61.710  41.578  1.00 12.72    A   O
ATOM   730 N   PRO A  95     36.728  61.263  42.765  1.00 14.67    A   N
ATOM   731 CD  PRO A  95     35.728  61.426  43.835  1.00 11.50    A   C
ATOM   732 CA  PRO A  95     36.612  59.933  42.154  1.00 13.49    A   C
ATOM   733 CB  PRO A  95     35.324  59.385  42.766  1.00 10.50    A   C
ATOM   734 CG  PRO A  95     35.340  59.990  44.132  1.00 13.67    A   C
ATOM   735 C   PRO A  95     36.552  59.995  40.628  1.00 13.36    A   C
ATOM   736 O   PRO A  95     37.111  59.144  39.942  1.00 13.11    A   O
ATOM   737 N   SER A  96     35.868  61.001  40.097  1.00 13.15    A   N
ATOM   738 CA  SER A  96     35.769  61.145  38.652  1.00 13.88    A   C
ATOM   739 CB  SER A  96     34.712  62.190  38.287  1.00 13.27    A   C
ATOM   740 OG  SER A  96     33.415  61.695  38.569  1.00 13.98    A   O
ATOM   741 C   SER A  96     37.121  61.532  38.062  1.00 16.13    A   C
ATOM   742 O   SER A  96     37.482  61.069  36.978  1.00 16.25    A   O
ATOM   743 N   ILE A  97     37.862  62.381  38.774  1.00 16.51    A   N
ATOM   744 CA  ILE A  97     39.181  62.807  38.318  1.00 16.84    A   C
ATOM   745 CB  ILE A  97     39.836  63.786  39.325  1.00 20.72    A   C
ATOM   746 CG2 ILE A  97     41.243  64.165  38.860  1.00 19.14    A   C
ATOM   747 CG1 ILE A  97     38.968  65.039  39.477  1.00 21.89    A   C
ATOM   748 CD1 ILE A  97     38.774  65.827  38.192  1.00 22.65    A   C
ATOM   749 C   ILE A  97     40.070  61.572  38.178  1.00 17.43    A   C
ATOM   750 O   ILE A  97     40.762  61.399  37.171  1.00 16.68    A   O
ATOM   751 N   LEU A  98     40.043  60.716  39.193  1.00 15.65    A   N
ATOM   752 CA  LEU A  98     40.840  59.498  39.182  1.00 18.16    A   C
ATOM   753 CB  LEU A  98     40.749  58.809  40.547  1.00 16.07    A   C
ATOM   754 CG  LEU A  98     41.359  59.641  41.682  1.00 15.84    A   C
ATOM   755 CD1 LEU A  98     41.069  58.980  43.020  1.00 13.47    A   C
ATOM   756 CD2 LEU A  98     42.866  59.788  41.466  1.00 19.12    A   C
ATOM   757 C   LEU A  98     40.374  58.563  38.063  1.00 17.77    A   C
ATOM   758 O   LEU A  98     41.199  57.934  37.389  1.00 16.62    A   O
ATOM   759 N   ALA A  99     39.058  58.485  37.859  1.00 16.23    A   N
ATOM   760 CA  ALA A  99     38.490  57.643  36.807  1.00 18.22    A   C
ATOM   761 CB  ALA A  99     36.962  57.767  36.788  1.00 20.22    A   C
ATOM   762 C   ALA A  99     39.065  58.077  35.462  1.00 17.90    A   C
ATOM   763 O   ALA A  99     39.496  57.246  34.658  1.00 17.01    A   O
ATOM   764 N   ILE A 100     39.067  59.386  35.226  1.00 15.73    A   N
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Figure 6O

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ATOM   765  CA  ILE A 100      39.601  59.939  33.987  1.00 17.26      A   C
ATOM   766  CB  ILE A 100      39.378  61.461  33.932  1.00 12.99      A   C
ATOM   767  CG2 ILE A 100      40.158  62.065  32.772  1.00 16.82      A   C
ATOM   768  CG1 ILE A 100      37.880  61.752  33.795  1.00 15.82      A   C
ATOM   769  CD1 ILE A 100      37.516  63.216  33.925  1.00 14.23      A   C
ATOM   770  C   ILE A 100      41.099  59.640  33.878  1.00 19.31      A   C
ATOM   771  O   ILE A 100      41.594  59.260  32.815  1.00 19.06      A   O
ATOM   772  N   LYS A 101      41.812  59.802  34.986  1.00 19.58      A   N
ATOM   773  CA  LYS A 101      43.246  59.543  35.019  1.00 22.07      A   C
ATOM   774  CB  LYS A 101      43.771  59.741  36.440  1.00 23.70      A   C
ATOM   775  CG  LYS A 101      45.273  59.581  36.595  1.00 28.63      A   C
ATOM   776  CD  LYS A 101      45.671  59.665  38.062  1.00 33.56      A   C
ATOM   777  CE  LYS A 101      47.180  59.570  38.245  1.00 36.39      A   C
ATOM   778  NZ  LYS A 101      47.894  60.739  37.649  1.00 38.26      A   N
ATOM   779  C   LYS A 101      43.538  58.117  34.551  1.00 23.93      A   C
ATOM   780  O   LYS A 101      44.472  57.882  33.780  1.00 23.77      A   O
ATOM   781  N   ARG A 102      42.723  57.174  35.010  1.00 23.37      A   N
ATOM   782  CA  ARG A 102      42.899  55.775  34.655  1.00 25.65      A   C
ATOM   783  CB  ARG A 102      42.096  54.870  35.593  1.00 25.41      A   C
ATOM   784  CG  ARG A 102      42.656  54.749  37.000  1.00 28.61      A   C
ATOM   785  CD  ARG A 102      41.926  53.657  37.782  1.00 31.73      A   C
ATOM   786  NE  ARG A 102      40.486  53.903  37.858  1.00 35.18      A   N
ATOM   787  CZ  ARG A 102      39.903  54.713  38.736  1.00 34.42      A   C
ATOM   788  NH1 ARG A 102      38.586  54.876  38.718  1.00 29.69      A   N
ATOM   789  NH2 ARG A 102      40.637  55.344  39.644  1.00 34.01      A   N
ATOM   790  C   ARG A 102      42.522  55.437  33.222  1.00 26.39      A   C
ATOM   791  O   ARG A 102      43.180  54.611  32.594  1.00 26.86      A   O
ATOM   792  N   GLN A 103      41.473  56.061  32.694  1.00 26.77      A   N
ATOM   793  CA  GLN A 103      41.067  55.733  31.331  1.00 27.82      A   C
ATOM   794  CB  GLN A 103      39.585  55.335  31.306  1.00 28.07      A   C
ATOM   795  CG  GLN A 103      38.661  56.210  32.116  1.00 31.66      A   C
ATOM   796  CD  GLN A 103      37.378  55.489  32.504  1.00 32.01      A   C
ATOM   797  OE1 GLN A 103      36.672  54.951  31.651  1.00 32.82      A   O
ATOM   798  NE2 GLN A 103      37.071  55.479  33.797  1.00 31.78      A   N
ATOM   799  C   GLN A 103      41.363  56.739  30.223  1.00 26.37      A   C
ATOM   800  O   GLN A 103      41.024  56.494  29.066  1.00 26.19      A   O
ATOM   801  N   VAL A 104      42.003  57.856  30.559  1.00 25.47      A   N
ATOM   802  CA  VAL A 104      42.342  58.855  29.550  1.00 24.55      A   C
ATOM   803  CB  VAL A 104      41.542  60.154  29.756  1.00 23.42      A   C
ATOM   804  CG1 VAL A 104      41.998  61.208  28.755  1.00 24.85      A   C
ATOM   805  CG2 VAL A 104      40.055  59.876  29.582  1.00 19.58      A   C
ATOM   806  C   VAL A 104      43.838  59.174  29.578  1.00 26.78      A   C
ATOM   807  O   VAL A 104      44.287  60.043  30.324  1.00 25.34      A   O
ATOM   808  N   GLU A 105      44.601  58.460  28.755  1.00 27.15      A   N
ATOM   809  CA  GLU A 105      46.045  58.641  28.679  1.00 28.29      A   C
ATOM   810  CB  GLU A 105      46.680  57.457  27.947  1.00 33.28      A   C
ATOM   811  CG  GLU A 105      46.743  56.183  28.771  1.00 42.55      A   C
ATOM   812  CD  GLU A 105      47.669  56.315  29.969  1.00 46.07      A   C
ATOM   813  OE1 GLU A 105      47.467  57.242  30.784  1.00 48.67      A   O
ATOM   814  OE2 GLU A 105      48.600  55.491  30.095  1.00 49.87      A   O
ATOM   815  C   GLU A 105      46.461  59.930  27.995  1.00 27.62      A   C
ATOM   816  O   GLU A 105      47.395  60.600  28.437  1.00 27.02      A   O
ATOM   817  N   ASP A 106      45.769  60.273  26.914  1.00 26.11      A   N
ATOM   818  CA  ASP A 106      46.079  61.485  26.164  1.00 25.35      A   C
ATOM   819  CB  ASP A 106      45.271  61.526  24.867  1.00 24.40      A   C
ATOM   820  CG  ASP A 106      45.714  62.641  23.932  1.00 25.06      A   C
ATOM   821  OD1 ASP A 106      46.302  63.640  24.404  1.00 25.51      A   O
ATOM   822  OD2 ASP A 106      45.458  62.522  22.718  1.00 25.51      A   O
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Figure 6P

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ATOM   823  C   ASP A 106     45.759  62.722  26.991  1.00 24.65      A   C
ATOM   824  O   ASP A 106     44.593  63.086  27.142  1.00 24.49      A   O
ATOM   825  N   LYS A 107     46.791  63.372  27.519  1.00 25.06      A   N
ATOM   826  CA  LYS A 107     46.593  64.570  28.327  1.00 24.62      A   C
ATOM   827  CB  LYS A 107     47.919  65.024  28.954  1.00 26.00      A   C
ATOM   828  CG  LYS A 107     48.506  64.047  29.972  1.00 28.40      A   C
ATOM   829  CD  LYS A 107     47.527  63.770  31.107  1.00 26.24      A   C
ATOM   830  CE  LYS A 107     48.086  62.757  32.090  1.00 30.72      A   C
ATOM   831  NZ  LYS A 107     47.086  62.398  33.133  1.00 34.82      A   N
ATOM   832  C   LYS A 107     46.000  65.708  27.503  1.00 24.04      A   C
ATOM   833  O   LYS A 107     45.538  66.706  28.054  1.00 25.01      A   O
ATOM   834  N   ASN A 108     46.014  65.555  26.182  1.00 24.07      A   N
ATOM   835  CA  ASN A 108     45.473  66.572  25.286  1.00 23.49      A   C
ATOM   836  CB  ASN A 108     46.390  66.750  24.073  1.00 23.91      A   C
ATOM   837  CG  ASN A 108     47.596  67.601  24.385  1.00 26.66      A   C
ATOM   838  OD1 ASN A 108     47.464  68.780  24.716  1.00 28.22      A   O
ATOM   839  ND2 ASN A 108     48.780  67.011  24.293  1.00 26.45      A   N
ATOM   840  C   ASN A 108     44.059  66.255  24.818  1.00 21.66      A   C
ATOM   841  O   ASN A 108     43.487  66.983  24.009  1.00 22.58      A   O
ATOM   842  N   ALA A 109     43.494  65.164  25.321  1.00 21.45      A   N
ATOM   843  CA  ALA A 109     42.137  64.793  24.946  1.00 20.49      A   C
ATOM   844  CB  ALA A 109     41.755  63.468  25.599  1.00 21.55      A   C
ATOM   845  C   ALA A 109     41.187  65.902  25.402  1.00 18.98      A   C
ATOM   846  O   ALA A 109     41.237  66.346  26.546  1.00 18.14      A   O
ATOM   847  N   PRO A 110     40.315  66.375  24.505  1.00 19.61      A   N
ATOM   848  CD  PRO A 110     40.090  65.997  23.100  1.00 20.78      A   C
ATOM   849  CA  PRO A 110     39.397  67.436  24.919  1.00 18.53      A   C
ATOM   850  CB  PRO A 110     38.762  67.872  23.606  1.00 18.56      A   C
ATOM   851  CG  PRO A 110     38.726  66.596  22.825  1.00 22.18      A   C
ATOM   852  C   PRO A 110     38.380  66.924  25.928  1.00 17.90      A   C
ATOM   853  O   PRO A 110     37.623  65.996  25.650  1.00 18.78      A   O
ATOM   854  N   ILE A 111     38.384  67.526  27.109  1.00 16.88      A   N
ATOM   855  CA  ILE A 111     37.461  67.137  28.165  1.00 16.87      A   C
ATOM   856  CB  ILE A 111     38.197  66.905  29.503  1.00 17.13      A   C
ATOM   857  CG2 ILE A 111     37.195  66.560  30.592  1.00 18.00      A   C
ATOM   858  CG1 ILE A 111     39.225  65.780  29.352  1.00 16.90      A   C
ATOM   859  CD1 ILE A 111     40.127  65.612  30.574  1.00 20.07      A   C
ATOM   860  C   ILE A 111     36.438  68.246  28.360  1.00 14.74      A   C
ATOM   861  O   ILE A 111     36.792  69.422  28.422  1.00 18.10      A   O
ATOM   862  N   LEU A 112     35.170  67.861  28.450  1.00 15.95      A   N
ATOM   863  CA  LEU A 112     34.086  68.814  28.646  1.00 15.98      A   C
ATOM   864  CB  LEU A 112     33.081  68.715  27.498  1.00 13.81      A   C
ATOM   865  CG  LEU A 112     31.755  69.460  27.703  1.00 17.30      A   C
ATOM   866  CD1 LEU A 112     32.000  70.958  27.834  1.00 12.50      A   C
ATOM   867  CD2 LEU A 112     30.832  69.165  26.524  1.00 17.57      A   C
ATOM   868  C   LEU A 112     33.379  68.527  29.966  1.00 15.50      A   C
ATOM   869  O   LEU A 112     32.823  67.445  30.158  1.00 14.25      A   O
ATOM   870  N   VAL A 113     33.394  69.507  30.864  1.00 15.54      A   N
ATOM   871  CA  VAL A 113     32.767  69.361  32.173  1.00 15.01      A   C
ATOM   872  CB  VAL A 113     33.614  70.035  33.278  1.00 16.33      A   C
ATOM   873  CG1 VAL A 113     33.011  69.752  34.653  1.00 12.34      A   C
ATOM   874  CG2 VAL A 113     35.053  69.538  33.208  1.00 15.51      A   C
ATOM   875  C   VAL A 113     31.390  70.006  32.178  1.00 15.47      A   C
ATOM   876  O   VAL A 113     31.257  71.197  31.901  1.00 15.67      A   O
ATOM   877  N   LEU A 114     30.370  69.215  32.494  1.00 14.67      A   N
ATOM   878  CA  LEU A 114     29.000  69.717  32.554  1.00 13.42      A   C
ATOM   879  CB  LEU A 114     28.074  68.836  31.716  1.00 13.87      A   C
ATOM   880  CG  LEU A 114     28.440  68.622  30.247  1.00 15.67      A   C
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Figure 6Q

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ATOM   881 CD1 LEU A 114     27.349  67.775  29.595  1.00 14.66    A   C
ATOM   882 CD2 LEU A 114     28.583  69.965  29.528  1.00 16.47    A   C
ATOM   883 C   LEU A 114     28.536  69.684  34.006  1.00 12.89    A   C
ATOM   884 O   LEU A 114     28.772  68.706  34.718  1.00 12.06    A   O
ATOM   885 N   GLY A 115     27.873  70.745  34.451  1.00 13.97    A   N
ATOM   886 CA  GLY A 115     27.403  70.763  35.822  1.00 12.19    A   C
ATOM   887 C   GLY A 115     26.528  71.961  36.088  1.00 13.28    A   C
ATOM   888 O   GLY A 115     26.171  72.696  35.160  1.00 14.73    A   O
ATOM   889 N   THR A 116     26.167  72.153  37.351  1.00 11.11    A   N
ATOM   890 CA  THR A 116     25.348  73.297  37.725  1.00 13.32    A   C
ATOM   891 CB  THR A 116     24.866  73.197  39.170  1.00 11.37    A   C
ATOM   892 OG1 THR A 116     26.000  73.180  40.041  1.00 10.70    A   O
ATOM   893 CG2 THR A 116     24.036  71.939  39.367  1.00 10.35    A   C
ATOM   894 C   THR A 116     26.195  74.554  37.614  1.00 14.14    A   C
ATOM   895 O   THR A 116     27.416  74.482  37.431  1.00 14.71    A   O
ATOM   896 N   LYS A 117     25.535  75.701  37.716  1.00 13.99    A   N
ATOM   897 CA  LYS A 117     26.204  76.993  37.657  1.00 14.71    A   C
ATOM   898 CB  LYS A 117     25.147  78.105  37.777  1.00 15.38    A   C
ATOM   899 CG  LYS A 117     25.652  79.472  38.236  1.00 25.83    A   C
ATOM   900 CD  LYS A 117     26.685  80.064  37.296  1.00 33.76    A   C
ATOM   901 CE  LYS A 117     26.103  80.361  35.920  1.00 38.20    A   C
ATOM   902 NZ  LYS A 117     27.105  81.002  35.015  1.00 42.09    A   N
ATOM   903 C   LYS A 117     27.233  77.085  38.787  1.00 12.72    A   C
ATOM   904 O   LYS A 117     28.356  77.549  38.588  1.00 11.82    A   O
ATOM   905 N   ALA A 118     26.854  76.621  39.972  1.00 11.59    A   N
ATOM   906 CA  ALA A 118     27.750  76.671  41.120  1.00 11.90    A   C
ATOM   907 CB  ALA A 118     26.990  76.297  42.382  1.00  8.77    A   C
ATOM   908 C   ALA A 118     28.965  75.758  40.955  1.00 13.39    A   C
ATOM   909 O   ALA A 118     30.099  76.161  41.223  1.00 14.34    A   O
ATOM   910 N   THR A 119     28.721  74.530  40.508  1.00 13.12    A   N
ATOM   911 CA  THR A 119     29.789  73.561  40.316  1.00 12.85    A   C
ATOM   912 CB  THR A 119     29.224  72.205  39.840  1.00 13.42    A   C
ATOM   913 OG1 THR A 119     28.398  71.647  40.869  1.00 11.57    A   O
ATOM   914 CG2 THR A 119     30.353  71.235  39.509  1.00 13.13    A   C
ATOM   915 C   THR A 119     30.808  74.050  39.298  1.00 12.99    A   C
ATOM   916 O   THR A 119     32.016  74.004  39.547  1.00 13.76    A   O
ATOM   917 N   ILE A 120     30.323  74.520  38.154  1.00 11.88    A   N
ATOM   918 CA  ILE A 120     31.213  75.003  37.103  1.00 13.74    A   C
ATOM   919 CB  ILE A 120     30.419  75.310  35.807  1.00 13.41    A   C
ATOM   920 CG2 ILE A 120     31.321  75.980  34.769  1.00 14.31    A   C
ATOM   921 CG1 ILE A 120     29.799  74.012  35.266  1.00 14.49    A   C
ATOM   922 CD1 ILE A 120     30.786  72.862  35.086  1.00 12.48    A   C
ATOM   923 C   ILE A 120     31.977  76.246  37.547  1.00 16.55    A   C
ATOM   924 O   ILE A 120     33.192  76.337  37.372  1.00 18.38    A   O
ATOM   925 N   GLN A 121     31.257  77.200  38.126  1.00 19.17    A   N
ATOM   926 CA  GLN A 121     31.861  78.437  38.601  1.00 20.47    A   C
ATOM   927 CB  GLN A 121     30.790  79.302  39.275  1.00 22.58    A   C
ATOM   928 CG  GLN A 121     31.332  80.406  40.175  1.00 27.23    A   C
ATOM   929 CD  GLN A 121     30.251  81.377  40.627  1.00 30.53    A   C
ATOM   930 OE1 GLN A 121     30.383  82.030  41.664  1.00 32.67    A   O
ATOM   931 NE2 GLN A 121     29.185  81.486  39.842  1.00 28.50    A   N
ATOM   932 C   GLN A 121     33.012  78.170  39.570  1.00 20.02    A   C
ATOM   933 O   GLN A 121     33.979  78.931  39.622  1.00 20.38    A   O
ATOM   934 N   SER A 122     32.905  77.082  40.326  1.00 20.65    A   N
ATOM   935 CA  SER A 122     33.919  76.709  41.311  1.00 19.01    A   C
ATOM   936 CB  SER A 122     33.377  75.609  42.222  1.00 17.57    A   C
ATOM   937 OG  SER A 122     33.446  74.356  41.556  1.00 13.49    A   O
ATOM   938 C   SER A 122     35.220  76.201  40.686  1.00 18.75    A   C
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Figure 6R

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ATOM   939  O   SER A 122     36.270  76.232  41.325  1.00 17.22      A   O
ATOM   940  N   ASN A 123     35.136  75.709  39.454  1.00 18.64      A   N
ATOM   941  CA  ASN A 123     36.292  75.159  38.752  1.00 19.81      A   C
ATOM   942  CB  ASN A 123     37.355  76.237  38.538  1.00 23.62      A   C
ATOM   943  CG  ASN A 123     36.915  77.277  37.537  1.00 27.79      A   C
ATOM   944  OD1 ASN A 123     36.375  76.939  36.483  1.00 25.00      A   O
ATOM   945  ND2 ASN A 123     37.141  78.549  37.855  1.00 30.06      A   N
ATOM   946  C   ASN A 123     36.898  73.967  39.487  1.00 18.35      A   C
ATOM   947  O   ASN A 123     38.057  73.606  39.272  1.00 15.93      A   O
ATOM   948  N   ALA A 124     36.101  73.356  40.356  1.00 16.83      A   N
ATOM   949  CA  ALA A 124     36.550  72.197  41.113  1.00 18.02      A   C
ATOM   950  CB  ALA A 124     35.392  71.613  41.914  1.00 17.02      A   C
ATOM   951  C   ALA A 124     37.109  71.148  40.157  1.00 16.55      A   C
ATOM   952  O   ALA A 124     38.195  70.614  40.376  1.00 17.86      A   O
ATOM   953  N   TYR A 125     36.370  70.858  39.091  1.00 15.55      A   N
ATOM   954  CA  TYR A 125     36.817  69.870  38.121  1.00 15.38      A   C
ATOM   955  CB  TYR A 125     35.699  69.549  37.125  1.00 14.36      A   C
ATOM   956  CG  TYR A 125     34.638  68.609  37.662  1.00 15.54      A   C
ATOM   957  CD1 TYR A 125     33.460  69.096  38.226  1.00 13.69      A   C
ATOM   958  CE1 TYR A 125     32.478  68.230  38.701  1.00 16.51      A   C
ATOM   959  CD2 TYR A 125     34.813  67.224  37.591  1.00 15.03      A   C
ATOM   960  CE2 TYR A 125     33.839  66.349  38.064  1.00 16.83      A   C
ATOM   961  CZ  TYR A 125     32.677  66.857  38.614  1.00 15.95      A   C
ATOM   962  OH  TYR A 125     31.718  65.993  39.065  1.00 16.50      A   O
ATOM   963  C   TYR A 125     38.060  70.323  37.361  1.00 15.65      A   C
ATOM   964  O   TYR A 125     39.050  69.596  37.289  1.00 12.18      A   O
ATOM   965  N   ASP A 126     37.998  71.523  36.796  1.00 15.04      A   N
ATOM   966  CA  ASP A 126     39.110  72.080  36.032  1.00 19.15      A   C
ATOM   967  CB  ASP A 126     38.805  73.530  35.642  1.00 18.87      A   C
ATOM   968  CG  ASP A 126     37.532  73.659  34.831  1.00 21.01      A   C
ATOM   969  OD1 ASP A 126     36.489  73.129  35.271  1.00 22.54      A   O
ATOM   970  OD2 ASP A 126     37.570  74.295  33.756  1.00 22.03      A   O
ATOM   971  C   ASP A 126     40.423  72.028  36.814  1.00 19.26      A   C
ATOM   972  O   ASP A 126     41.432  71.519  36.316  1.00 19.31      A   O
ATOM   973  N   ASN A 127     40.406  72.542  38.040  1.00 18.32      A   N
ATOM   974  CA  ASN A 127     41.613  72.549  38.860  1.00 20.39      A   C
ATOM   975  CB  ASN A 127     41.349  73.226  40.206  1.00 19.27      A   C
ATOM   976  CG  ASN A 127     41.031  74.703  40.067  1.00 23.43      A   C
ATOM   977  OD1 ASN A 127     41.553  75.382  39.185  1.00 25.20      A   O
ATOM   978  ND2 ASN A 127     40.185  75.213  40.955  1.00 22.93      A   N
ATOM   979  C   ASN A 127     42.183  71.155  39.096  1.00 19.69      A   C
ATOM   980  O   ASN A 127     43.381  70.926  38.926  1.00 19.93      A   O
ATOM   981  N   ALA A 128     41.325  70.222  39.488  1.00 17.80      A   N
ATOM   982  CA  ALA A 128     41.767  68.862  39.742  1.00 19.25      A   C
ATOM   983  CB  ALA A 128     40.596  68.016  40.218  1.00 17.14      A   C
ATOM   984  C   ALA A 128     42.383  68.253  38.489  1.00 18.99      A   C
ATOM   985  O   ALA A 128     43.434  67.614  38.553  1.00 21.03      A   O
ATOM   986  N   LEU A 129     41.734  68.456  37.347  1.00 18.35      A   N
ATOM   987  CA  LEU A 129     42.237  67.911  36.088  1.00 18.37      A   C
ATOM   988  CB  LEU A 129     41.229  68.157  34.966  1.00 16.99      A   C
ATOM   989  CG  LEU A 129     39.944  67.331  35.044  1.00 17.37      A   C
ATOM   990  CD1 LEU A 129     38.906  67.908  34.101  1.00 18.55      A   C
ATOM   991  CD2 LEU A 129     40.247  65.878  34.690  1.00 19.31      A   C
ATOM   992  C   LEU A 129     43.586  68.512  35.709  1.00 18.69      A   C
ATOM   993  O   LEU A 129     44.486  67.799  35.264  1.00 16.61      A   O
ATOM   994  N   LYS A 130     43.722  69.823  35.881  1.00 20.51      A   N
ATOM   995  CA  LYS A 130     44.974  70.492  35.559  1.00 25.95      A   C
ATOM   996  CB  LYS A 130     44.869  72.002  35.815  1.00 29.56      A   C
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Figure 6S

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ATOM   997 CG  LYS A 130    44.065  72.756  34.766  1.00 35.38    A   C
ATOM   998 CD  LYS A 130    44.211  74.273  34.910  1.00 40.67    A   C
ATOM   999 CE  LYS A 130    43.491  74.796  36.138  1.00 44.58    A   C
ATOM  1000 NZ  LYS A 130    42.021  74.573  36.036  1.00 48.51    A   N
ATOM  1001 C   LYS A 130    46.084  69.899  36.413  1.00 27.20    A   C
ATOM  1002 O   LYS A 130    47.173  69.607  35.921  1.00 26.83    A   O
ATOM  1003 N   GLN A 131    45.793  69.711  37.695  1.00 27.73    A   N
ATOM  1004 CA  GLN A 131    46.768  69.152  38.615  1.00 30.51    A   C
ATOM  1005 CB  GLN A 131    46.168  69.058  40.017  1.00 34.61    A   C
ATOM  1006 CG  GLN A 131    47.164  68.658  41.086  1.00 44.44    A   C
ATOM  1007 CD  GLN A 131    46.499  68.364  42.414  1.00 49.85    A   C
ATOM  1008 OE1 GLN A 131    45.721  67.415  42.532  1.00 53.57    A   O
ATOM  1009 NE2 GLN A 131    46.797  69.181  43.423  1.00 52.59    A   N
ATOM  1010 C   GLN A 131    47.205  67.769  38.139  1.00 29.59    A   C
ATOM  1011 O   GLN A 131    48.333  67.347  38.389  1.00 27.34    A   O
ATOM  1012 N   GLN A 132    46.311  67.066  37.452  1.00 27.34    A   N
ATOM  1013 CA  GLN A 132    46.634  65.738  36.950  1.00 28.50    A   C
ATOM  1014 CB  GLN A 132    45.382  64.865  36.894  1.00 30.13    A   C
ATOM  1015 CG  GLN A 132    44.863  64.445  38.253  1.00 32.88    A   C
ATOM  1016 CD  GLN A 132    45.924  63.758  39.093  1.00 36.97    A   C
ATOM  1017 OE1 GLN A 132    46.545  62.787  38.659  1.00 36.12    A   O
ATOM  1018 NE2 GLN A 132    46.136  64.262  40.308  1.00 36.40    A   N
ATOM  1019 C   GLN A 132    47.297  65.764  35.579  1.00 26.54    A   C
ATOM  1020 O   GLN A 132    47.465  64.721  34.948  1.00 25.99    A   O
ATOM  1021 N   GLY A 133    47.653  66.958  35.113  1.00 25.65    A   N
ATOM  1022 CA  GLY A 133    48.326  67.079  33.833  1.00 25.61    A   C
ATOM  1023 C   GLY A 133    47.496  67.252  32.575  1.00 26.98    A   C
ATOM  1024 O   GLY A 133    48.061  67.293  31.479  1.00 25.64    A   O
ATOM  1025 N   TYR A 134    46.174  67.353  32.696  1.00 25.10    A   N
ATOM  1026 CA  TYR A 134    45.357  67.526  31.495  1.00 24.59    A   C
ATOM  1027 CB  TYR A 134    43.902  67.120  31.762  1.00 20.44    A   C
ATOM  1028 CG  TYR A 134    43.781  65.626  31.951  1.00 19.78    A   C
ATOM  1029 CD1 TYR A 134    43.870  65.050  33.219  1.00 21.76    A   C
ATOM  1030 CE1 TYR A 134    43.868  63.664  33.380  1.00 19.57    A   C
ATOM  1031 CD2 TYR A 134    43.681  64.774  30.850  1.00 19.08    A   C
ATOM  1032 CE2 TYR A 134    43.682  63.389  31.002  1.00 17.24    A   C
ATOM  1033 CZ  TYR A 134    43.777  62.842  32.265  1.00 18.47    A   C
ATOM  1034 OH  TYR A 134    43.792  61.473  32.413  1.00 19.23    A   O
ATOM  1035 C   TYR A 134    45.461  68.951  30.972  1.00 22.87    A   C
ATOM  1036 O   TYR A 134    45.446  69.908  31.746  1.00 22.48    A   O
ATOM  1037 N   LEU A 135    45.571  69.078  29.650  1.00 22.86    A   N
ATOM  1038 CA  LEU A 135    45.750  70.377  29.008  1.00 24.08    A   C
ATOM  1039 CB  LEU A 135    47.048  70.359  28.192  1.00 24.76    A   C
ATOM  1040 CG  LEU A 135    48.311  69.857  28.906  1.00 25.95    A   C
ATOM  1041 CD1 LEU A 135    49.461  69.790  27.913  1.00 27.98    A   C
ATOM  1042 CD2 LEU A 135    48.658  70.779  30.068  1.00 26.13    A   C
ATOM  1043 C   LEU A 135    44.628  70.873  28.107  1.00 23.53    A   C
ATOM  1044 O   LEU A 135    44.736  71.957  27.539  1.00 24.90    A   O
ATOM  1045 N   ASN A 136    43.556  70.100  27.970  1.00 22.37    A   N
ATOM  1046 CA  ASN A 136    42.450  70.499  27.102  1.00 20.74    A   C
ATOM  1047 CB  ASN A 136    42.411  69.585  25.876  1.00 21.50    A   C
ATOM  1048 CG  ASN A 136    41.613  70.170  24.735  1.00 23.18    A   C
ATOM  1049 OD1 ASN A 136    40.590  70.822  24.945  1.00 25.29    A   O
ATOM  1050 ND2 ASN A 136    42.068  69.923  23.511  1.00 23.17    A   N
ATOM  1051 C   ASN A 136    41.146  70.370  27.887  1.00 20.55    A   C
ATOM  1052 O   ASN A 136    40.430  69.386  27.744  1.00 20.93    A   O
ATOM  1053 N   ILE A 137    40.847  71.371  28.709  1.00 19.65    A   N
ATOM  1054 CA  ILE A 137    39.649  71.347  29.545  1.00 19.51    A   C
```

Figure 6T

ATOM 1055 CB ILE A 137 40.021 71.504 31.032 1.00 19.77 A C
ATOM 1056 CG2 ILE A 137 38.792 71.235 31.905 1.00 18.91 A C
ATOM 1057 CG1 ILE A 137 41.165 70.548 31.388 1.00 17.50 A C
ATOM 1058 CD1 ILE A 137 41.841 70.877 32.705 1.00 17.99 A C
ATOM 1059 C ILE A 137 38.650 72.445 29.214 1.00 18.94 A C
ATOM 1060 O ILE A 137 39.008 73.618 29.141 1.00 18.47 A O
ATOM 1061 N SER A 138 37.394 72.054 29.019 1.00 18.59 A N
ATOM 1062 CA SER A 138 36.319 73.000 28.729 1.00 19.77 A C
ATOM 1063 CB SER A 138 35.810 72.829 27.294 1.00 21.73 A C
ATOM 1064 OG SER A 138 36.823 73.104 26.345 1.00 24.47 A O
ATOM 1065 C SER A 138 35.177 72.716 29.698 1.00 19.64 A C
ATOM 1066 O SER A 138 34.971 71.569 30.102 1.00 20.10 A O
ATOM 1067 N HIS A 139 34.443 73.753 30.083 1.00 18.51 A N
ATOM 1068 CA HIS A 139 33.319 73.565 30.993 1.00 18.98 A C
ATOM 1069 CB HIS A 139 33.697 73.982 32.418 1.00 18.17 A C
ATOM 1070 CG HIS A 139 34.220 75.380 32.522 1.00 19.94 A C
ATOM 1071 CD2 HIS A 139 33.634 76.575 32.268 1.00 20.85 A C
ATOM 1072 ND1 HIS A 139 35.506 75.661 32.926 1.00 20.98 A N
ATOM 1073 CE1 HIS A 139 35.692 76.970 32.916 1.00 24.03 A C
ATOM 1074 NE2 HIS A 139 34.572 77.547 32.520 1.00 22.03 A N
ATOM 1075 C HIS A 139 32.082 74.329 30.552 1.00 18.46 A C
ATOM 1076 O HIS A 139 32.181 75.372 29.909 1.00 19.58 A O
ATOM 1077 N LEU A 140 30.918 73.791 30.902 1.00 18.71 A N
ATOM 1078 CA LEU A 140 29.634 74.403 30.573 1.00 19.01 A C
ATOM 1079 CB LEU A 140 29.028 73.775 29.316 1.00 20.85 A C
ATOM 1080 CG LEU A 140 29.476 74.190 27.918 1.00 22.92 A C
ATOM 1081 CD1 LEU A 140 28.667 73.394 26.904 1.00 21.79 A C
ATOM 1082 CD2 LEU A 140 29.255 75.688 27.709 1.00 25.42 A C
ATOM 1083 C LEU A 140 28.632 74.227 31.702 1.00 17.69 A C
ATOM 1084 O LEU A 140 28.422 73.118 32.194 1.00 17.06 A O
ATOM 1085 N ALA A 141 28.008 75.322 32.112 1.00 18.99 A N
ATOM 1086 CA ALA A 141 26.995 75.256 33.153 1.00 18.92 A C
ATOM 1087 CB ALA A 141 26.976 76.553 33.955 1.00 19.92 A C
ATOM 1088 C ALA A 141 25.653 75.046 32.456 1.00 20.05 A C
ATOM 1089 O ALA A 141 25.002 76.007 32.053 1.00 22.92 A O
ATOM 1090 N THR A 142 25.250 73.790 32.299 1.00 17.67 A N
ATOM 1091 CA THR A 142 23.983 73.456 31.650 1.00 15.92 A C
ATOM 1092 CB THR A 142 24.069 72.061 30.991 1.00 15.55 A C
ATOM 1093 OG1 THR A 142 24.474 71.094 31.969 1.00 15.28 A O
ATOM 1094 CG2 THR A 142 25.091 72.069 29.862 1.00 16.16 A C
ATOM 1095 C THR A 142 22.890 73.462 32.725 1.00 16.51 A C
ATOM 1096 O THR A 142 22.195 72.469 32.942 1.00 15.07 A O
ATOM 1097 N SER A 143 22.746 74.608 33.382 1.00 15.40 A N
ATOM 1098 CA SER A 143 21.797 74.779 34.479 1.00 16.69 A C
ATOM 1099 CB SER A 143 21.745 76.254 34.886 1.00 18.40 A C
ATOM 1100 OG SER A 143 20.979 76.419 36.068 1.00 19.14 A O
ATOM 1101 C SER A 143 20.374 74.259 34.266 1.00 16.28 A C
ATOM 1102 O SER A 143 19.838 73.555 35.119 1.00 17.50 A O
ATOM 1103 N LEU A 144 19.766 74.597 33.133 1.00 15.61 A N
ATOM 1104 CA LEU A 144 18.397 74.174 32.850 1.00 16.29 A C
ATOM 1105 CB LEU A 144 17.920 74.855 31.567 1.00 18.23 A C
ATOM 1106 CG LEU A 144 17.915 76.379 31.743 1.00 21.65 A C
ATOM 1107 CD1 LEU A 144 17.543 77.079 30.440 1.00 21.02 A C
ATOM 1108 CD2 LEU A 144 16.931 76.741 32.854 1.00 19.77 A C
ATOM 1109 C LEU A 144 18.171 72.657 32.772 1.00 15.16 A C
ATOM 1110 O LEU A 144 17.036 72.184 32.874 1.00 13.64 A O
ATOM 1111 N PHE A 145 19.238 71.888 32.600 1.00 13.93 A N
ATOM 1112 CA PHE A 145 19.080 70.437 32.545 1.00 11.95 A C

Figure 6U

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ATOM  1113  CB  PHE A 145      20.436  69.742  32.374  1.00 13.43      A   C
ATOM  1114  CG  PHE A 145      21.000  69.808  30.976  1.00 17.43      A   C
ATOM  1115  CD1 PHE A 145      22.248  69.260  30.703  1.00 15.45      A   C
ATOM  1116  CD2 PHE A 145      20.287  70.399  29.933  1.00 17.04      A   C
ATOM  1117  CE1 PHE A 145      22.783  69.295  29.420  1.00 18.35      A   C
ATOM  1118  CE2 PHE A 145      20.815  70.440  28.642  1.00 15.38      A   C
ATOM  1119  CZ  PHE A 145      22.064  69.889  28.385  1.00 16.89      A   C
ATOM  1120  C   PHE A 145      18.436  69.956  33.846  1.00 12.03      A   C
ATOM  1121  O   PHE A 145      17.600  69.064  33.839  1.00 11.95      A   O
ATOM  1122  N   VAL A 146      18.813  70.564  34.965  1.00 12.43      A   N
ATOM  1123  CA  VAL A 146      18.269  70.150  36.255  1.00 11.55      A   C
ATOM  1124  CB  VAL A 146      18.931  70.941  37.420  1.00 11.44      A   C
ATOM  1125  CG1 VAL A 146      18.203  70.669  38.739  1.00 12.27      A   C
ATOM  1126  CG2 VAL A 146      20.389  70.523  37.541  1.00 12.17      A   C
ATOM  1127  C   VAL A 146      16.741  70.243  36.344  1.00 13.17      A   C
ATOM  1128  O   VAL A 146      16.081  69.236  36.566  1.00 13.35      A   O
ATOM  1129  N   PRO A 147      16.157  71.442  36.168  1.00 14.55      A   N
ATOM  1130  CD  PRO A 147      16.725  72.794  36.014  1.00 12.51      A   C
ATOM  1131  CA  PRO A 147      14.693  71.491  36.260  1.00 15.45      A   C
ATOM  1132  CB  PRO A 147      14.386  72.995  36.197  1.00 16.91      A   C
ATOM  1133  CG  PRO A 147      15.556  73.569  35.463  1.00 13.21      A   C
ATOM  1134  C   PRO A 147      13.972  70.682  35.178  1.00 13.90      A   C
ATOM  1135  O   PRO A 147      12.910  70.111  35.433  1.00 15.62      A   O
ATOM  1136  N   LEU A 148      14.549  70.614  33.982  1.00 11.79      A   N
ATOM  1137  CA  LEU A 148      13.929  69.844  32.911  1.00 13.83      A   C
ATOM  1138  CB  LEU A 148      14.748  69.947  31.620  1.00 15.89      A   C
ATOM  1139  CG  LEU A 148      14.193  70.877  30.540  1.00 14.82      A   C
ATOM  1140  CD1 LEU A 148      14.146  72.296  31.057  1.00 18.80      A   C
ATOM  1141  CD2 LEU A 148      15.070  70.792  29.300  1.00 16.16      A   C
ATOM  1142  C   LEU A 148      13.833  68.389  33.336  1.00 13.84      A   C
ATOM  1143  O   LEU A 148      12.786  67.755  33.204  1.00 15.22      A   O
ATOM  1144  N   ILE A 149      14.935  67.872  33.861  1.00 12.81      A   N
ATOM  1145  CA  ILE A 149      14.985  66.493  34.312  1.00 13.21      A   C
ATOM  1146  CB  ILE A 149      16.425  66.111  34.703  1.00 14.51      A   C
ATOM  1147  CG2 ILE A 149      16.444  64.756  35.402  1.00 12.63      A   C
ATOM  1148  CG1 ILE A 149      17.291  66.093  33.434  1.00 15.10      A   C
ATOM  1149  CD1 ILE A 149      18.777  65.893  33.673  1.00 10.57      A   C
ATOM  1150  C   ILE A 149      14.026  66.258  35.470  1.00 14.45      A   C
ATOM  1151  O   ILE A 149      13.425  65.195  35.571  1.00 15.79      A   O
ATOM  1152  N   GLU A 150      13.859  67.256  36.328  1.00 14.06      A   N
ATOM  1153  CA  GLU A 150      12.943  67.121  37.449  1.00 15.01      A   C
ATOM  1154  CB  GLU A 150      13.206  68.228  38.466  1.00 18.77      A   C
ATOM  1155  CG  GLU A 150      14.447  67.930  39.291  1.00 26.06      A   C
ATOM  1156  CD  GLU A 150      14.824  69.044  40.227  1.00 28.16      A   C
ATOM  1157  OE1 GLU A 150      15.731  68.821  41.056  1.00 26.46      A   O
ATOM  1158  OE2 GLU A 150      14.222  70.138  40.128  1.00 31.52      A   O
ATOM  1159  C   GLU A 150      11.481  67.116  37.000  1.00 15.40      A   C
ATOM  1160  O   GLU A 150      10.615  66.617  37.719  1.00 14.17      A   O
ATOM  1161  N   GLU A 151      11.212  67.680  35.822  1.00 13.23      A   N
ATOM  1162  CA  GLU A 151       9.860  67.703  35.265  1.00 15.55      A   C
ATOM  1163  CB  GLU A 151       9.619  68.971  34.442  1.00 16.54      A   C
ATOM  1164  CG  GLU A 151       9.533  70.248  35.267  1.00 20.37      A   C
ATOM  1165  CD  GLU A 151       8.528  70.151  36.401  1.00 23.39      A   C
ATOM  1166  OE1 GLU A 151       7.332  69.901  36.134  1.00 24.54      A   O
ATOM  1167  OE2 GLU A 151       8.937  70.326  37.566  1.00 27.18      A   O
ATOM  1168  C   GLU A 151       9.687  66.487  34.368  1.00 17.22      A   C
ATOM  1169  O   GLU A 151       8.668  66.331  33.687  1.00 16.37      A   O
ATOM  1170  N   SER A 152      10.702  65.632  34.376  1.00 18.04      A   N
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Figure 6V

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ATOM  1171  CA  SER A 152      10.722  64.413  33.578  1.00 18.02      A   C
ATOM  1172  CB  SER A 152       9.559  63.493  33.949  1.00 19.94      A   C
ATOM  1173  OG  SER A 152       9.768  62.207  33.390  1.00 18.81      A   O
ATOM  1174  C   SER A 152      10.699  64.673  32.081  1.00 20.44      A   C
ATOM  1175  O   SER A 152      10.013  63.980  31.323  1.00 22.59      A   O
ATOM  1176  N   ILE A 153      11.443  65.682  31.653  1.00 19.73      A   N
ATOM  1177  CA  ILE A 153      11.541  65.998  30.239  1.00 21.13      A   C
ATOM  1178  CB  ILE A 153      11.541  67.521  30.016  1.00 23.26      A   C
ATOM  1179  CG2 ILE A 153      11.800  67.846  28.546  1.00 22.78      A   C
ATOM  1180  CG1 ILE A 153      10.190  68.086  30.474  1.00 25.17      A   C
ATOM  1181  CD1 ILE A 153      10.005  69.547  30.207  1.00 30.23      A   C
ATOM  1182  C   ILE A 153      12.865  65.372  29.832  1.00 21.67      A   C
ATOM  1183  O   ILE A 153      13.900  66.037  29.784  1.00 20.32      A   O
ATOM  1184  N   LEU A 154      12.811  64.069  29.565  1.00 18.75      A   N
ATOM  1185  CA  LEU A 154      13.986  63.281  29.218  1.00 20.85      A   C
ATOM  1186  CB  LEU A 154      13.939  61.972  30.003  1.00 21.22      A   C
ATOM  1187  CG  LEU A 154      13.540  62.197  31.467  1.00 22.53      A   C
ATOM  1188  CD1 LEU A 154      13.353  60.868  32.182  1.00 21.31      A   C
ATOM  1189  CD2 LEU A 154      14.604  63.040  32.154  1.00 20.71      A   C
ATOM  1190  C   LEU A 154      14.131  62.994  27.726  1.00 21.27      A   C
ATOM  1191  O   LEU A 154      14.969  62.194  27.313  1.00 20.75      A   O
ATOM  1192  N   GLU A 155      13.302  63.649  26.927  1.00 23.77      A   N
ATOM  1193  CA  GLU A 155      13.333  63.499  25.478  1.00 26.10      A   C
ATOM  1194  CB  GLU A 155      12.948  62.069  25.074  1.00 30.66      A   C
ATOM  1195  CG  GLU A 155      11.661  61.554  25.686  1.00 38.37      A   C
ATOM  1196  CD  GLU A 155      10.445  61.898  24.860  1.00 42.76      A   C
ATOM  1197  OE1 GLU A 155       9.322  61.571  25.299  1.00 48.12      A   O
ATOM  1198  OE2 GLU A 155      10.609  62.488  23.771  1.00 46.52      A   O
ATOM  1199  C   GLU A 155      12.366  64.517  24.893  1.00 24.72      A   C
ATOM  1200  O   GLU A 155      11.759  65.288  25.633  1.00 23.59      A   O
ATOM  1201  N   GLY A 156      12.236  64.538  23.573  1.00 23.02      A   N
ATOM  1202  CA  GLY A 156      11.333  65.492  22.958  1.00 21.08      A   C
ATOM  1203  C   GLY A 156      12.047  66.742  22.485  1.00 22.30      A   C
ATOM  1204  O   GLY A 156      13.243  66.925  22.728  1.00 21.15      A   O
ATOM  1205  N   GLU A 157      11.299  67.612  21.817  1.00 20.99      A   N
ATOM  1206  CA  GLU A 157      11.847  68.844  21.268  1.00 22.12      A   C
ATOM  1207  CB  GLU A 157      10.786  69.539  20.412  1.00 25.41      A   C
ATOM  1208  CG  GLU A 157      11.366  70.505  19.398  1.00 32.26      A   C
ATOM  1209  CD  GLU A 157      10.304  71.341  18.720  1.00 37.00      A   C
ATOM  1210  OE1 GLU A 157       9.332  70.758  18.186  1.00 41.42      A   O
ATOM  1211  OE2 GLU A 157      10.443  72.583  18.719  1.00 39.91      A   O
ATOM  1212  C   GLU A 157      12.386  69.835  22.302  1.00 19.65      A   C
ATOM  1213  O   GLU A 157      13.377  70.518  22.053  1.00 18.65      A   O
ATOM  1214  N   LEU A 158      11.734  69.925  23.453  1.00 18.49      A   N
ATOM  1215  CA  LEU A 158      12.172  70.861  24.485  1.00 20.02      A   C
ATOM  1216  CB  LEU A 158      11.174  70.870  25.653  1.00 19.53      A   C
ATOM  1217  CG  LEU A 158      11.410  71.891  26.773  1.00 21.01      A   C
ATOM  1218  CD1 LEU A 158      11.661  73.280  26.191  1.00 20.32      A   C
ATOM  1219  CD2 LEU A 158      10.197  71.910  27.697  1.00 19.63      A   C
ATOM  1220  C   LEU A 158      13.581  70.529  24.976  1.00 17.50      A   C
ATOM  1221  O   LEU A 158      14.424  71.417  25.101  1.00 17.99      A   O
ATOM  1222  N   LEU A 159      13.846  69.253  25.240  1.00 18.72      A   N
ATOM  1223  CA  LEU A 159      15.180  68.856  25.693  1.00 17.84      A   C
ATOM  1224  CB  LEU A 159      15.202  67.377  26.105  1.00 17.62      A   C
ATOM  1225  CG  LEU A 159      16.585  66.818  26.488  1.00 16.01      A   C
ATOM  1226  CD1 LEU A 159      17.125  67.557  27.713  1.00 16.76      A   C
ATOM  1227  CD2 LEU A 159      16.478  65.324  26.775  1.00 16.92      A   C
ATOM  1228  C   LEU A 159      16.185  69.091  24.571  1.00 18.06      A   C
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Figure 6W

ATOM 1229 O LEU A 159 17.274 69.629 24.792 1.00 15.90 A O
ATOM 1230 N GLU A 160 15.805 68.686 23.363 1.00 17.23 A N
ATOM 1231 CA GLU A 160 16.660 68.846 22.199 1.00 19.74 A C
ATOM 1232 CB GLU A 160 15.936 68.322 20.951 1.00 22.63 A C
ATOM 1233 CG GLU A 160 16.613 68.624 19.612 1.00 25.09 A C
ATOM 1234 CD GLU A 160 18.020 68.058 19.496 1.00 28.46 A C
ATOM 1235 OE1 GLU A 160 18.320 67.041 20.156 1.00 24.99 A O
ATOM 1236 OE2 GLU A 160 18.824 68.626 18.725 1.00 29.33 A O
ATOM 1237 C GLU A 160 17.025 70.316 22.023 1.00 17.75 A C
ATOM 1238 O GLU A 160 18.188 70.655 21.795 1.00 17.75 A O
ATOM 1239 N THR A 161 16.031 71.188 22.140 1.00 15.91 A N
ATOM 1240 CA THR A 161 16.274 72.615 21.984 1.00 17.08 A C
ATOM 1241 CB THR A 161 14.955 73.402 21.946 1.00 19.03 A C
ATOM 1242 OG1 THR A 161 14.165 72.943 20.841 1.00 18.83 A O
ATOM 1243 CG2 THR A 161 15.225 74.888 21.770 1.00 18.63 A C
ATOM 1244 C THR A 161 17.159 73.154 23.104 1.00 16.80 A C
ATOM 1245 O THR A 161 17.998 74.029 22.875 1.00 16.81 A O
ATOM 1246 N CYS A 162 16.977 72.623 24.309 1.00 15.47 A N
ATOM 1247 CA CYS A 162 17.772 73.054 25.451 1.00 16.48 A C
ATOM 1248 CB CYS A 162 17.217 72.456 26.748 1.00 17.44 A C
ATOM 1249 SG CYS A 162 17.994 73.125 28.246 1.00 17.16 A S
ATOM 1250 C CYS A 162 19.226 72.624 25.264 1.00 16.12 A C
ATOM 1251 O CYS A 162 20.148 73.390 25.547 1.00 15.64 A O
ATOM 1252 N MET A 163 19.433 71.395 24.797 1.00 16.12 A N
ATOM 1253 CA MET A 163 20.792 70.913 24.578 1.00 16.90 A C
ATOM 1254 CB MET A 163 20.796 69.446 24.152 1.00 17.54 A C
ATOM 1255 CG MET A 163 20.259 68.491 25.198 1.00 18.15 A C
ATOM 1256 SD MET A 163 20.679 66.775 24.864 1.00 18.78 A S
ATOM 1257 CE MET A 163 19.539 66.408 23.514 1.00 18.51 A C
ATOM 1258 C MET A 163 21.427 71.760 23.483 1.00 16.80 A C
ATOM 1259 O MET A 163 22.601 72.109 23.554 1.00 17.90 A O
ATOM 1260 N HIS A 164 20.637 72.083 22.467 1.00 17.35 A N
ATOM 1261 CA HIS A 164 21.119 72.893 21.359 1.00 18.77 A C
ATOM 1262 CB HIS A 164 20.009 73.065 20.317 1.00 21.03 A C
ATOM 1263 CG HIS A 164 20.451 73.784 19.082 1.00 26.61 A C
ATOM 1264 CD2 HIS A 164 20.862 73.317 17.879 1.00 27.02 A C
ATOM 1265 ND1 HIS A 164 20.559 75.156 19.018 1.00 26.82 A N
ATOM 1266 CE1 HIS A 164 21.020 75.503 17.829 1.00 28.20 A C
ATOM 1267 NE2 HIS A 164 21.212 74.406 17.119 1.00 26.69 A N
ATOM 1268 C HIS A 164 21.573 74.249 21.872 1.00 17.93 A C
ATOM 1269 O HIS A 164 22.630 74.758 21.483 1.00 18.32 A O
ATOM 1270 N TYR A 165 20.775 74.821 22.765 1.00 16.78 A N
ATOM 1271 CA TYR A 165 21.073 76.120 23.352 1.00 17.03 A C
ATOM 1272 CB TYR A 165 20.004 76.486 24.383 1.00 16.70 A C
ATOM 1273 CG TYR A 165 20.323 77.728 25.186 1.00 14.36 A C
ATOM 1274 CD1 TYR A 165 20.249 78.998 24.611 1.00 18.03 A C
ATOM 1275 CE1 TYR A 165 20.567 80.144 25.350 1.00 17.68 A C
ATOM 1276 CD2 TYR A 165 20.722 77.633 26.518 1.00 15.98 A C
ATOM 1277 CE2 TYR A 165 21.042 78.767 27.263 1.00 15.67 A C
ATOM 1278 CZ TYR A 165 20.964 80.015 26.675 1.00 17.67 A C
ATOM 1279 OH TYR A 165 21.296 81.128 27.414 1.00 19.35 A O
ATOM 1280 C TYR A 165 22.440 76.144 24.025 1.00 18.18 A C
ATOM 1281 O TYR A 165 23.202 77.089 23.848 1.00 18.56 A O
ATOM 1282 N TYR A 166 22.745 75.101 24.795 1.00 16.65 A N
ATOM 1283 CA TYR A 166 24.016 75.022 25.516 1.00 16.14 A C
ATOM 1284 CB TYR A 166 23.879 74.113 26.745 1.00 15.22 A C
ATOM 1285 CG TYR A 166 23.063 74.681 27.887 1.00 14.44 A C
ATOM 1286 CD1 TYR A 166 21.955 73.994 28.380 1.00 13.39 A C

Figure 6X

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ATOM  1287  CE1 TYR A 166     21.202  74.506  29.438  1.00 14.31      A   C
ATOM  1288  CD2 TYR A 166     23.403  75.898  28.481  1.00 14.07      A   C
ATOM  1289  CE2 TYR A 166     22.660  76.419  29.537  1.00 13.27      A   C
ATOM  1290  CZ  TYR A 166     21.558  75.717  30.008  1.00 15.59      A   C
ATOM  1291  OH  TYR A 166     20.800  76.228  31.033  1.00 13.70      A   O
ATOM  1292  C   TYR A 166     25.207  74.520  24.710  1.00 16.15      A   C
ATOM  1293  O   TYR A 166     26.320  75.020  24.862  1.00 18.32      A   O
ATOM  1294  N   PHE A 167     24.977  73.532  23.858  1.00 16.40      A   N
ATOM  1295  CA  PHE A 167     26.063  72.926  23.099  1.00 19.32      A   C
ATOM  1296  CB  PHE A 167     25.696  71.466  22.811  1.00 18.55      A   C
ATOM  1297  CG  PHE A 167     25.487  70.633  24.056  1.00 17.57      A   C
ATOM  1298  CD1 PHE A 167     24.611  69.551  24.044  1.00 17.73      A   C
ATOM  1299  CD2 PHE A 167     26.179  70.920  25.232  1.00 17.53      A   C
ATOM  1300  CE1 PHE A 167     24.429  68.766  25.186  1.00 17.59      A   C
ATOM  1301  CE2 PHE A 167     26.005  70.140  26.378  1.00 15.09      A   C
ATOM  1302  CZ  PHE A 167     25.130  69.063  26.354  1.00 15.31      A   C
ATOM  1303  C   PHE A 167     26.517  73.613  21.810  1.00 21.91      A   C
ATOM  1304  O   PHE A 167     27.693  73.529  21.444  1.00 18.63      A   O
ATOM  1305  N   THR A 168     25.600  74.293  21.128  1.00 23.53      A   N
ATOM  1306  CA  THR A 168     25.940  74.958  19.871  1.00 25.11      A   C
ATOM  1307  CB  THR A 168     24.757  75.788  19.346  1.00 24.47      A   C
ATOM  1308  OG1 THR A 168     23.646  74.919  19.099  1.00 28.03      A   O
ATOM  1309  CG2 THR A 168     25.133  76.488  18.048  1.00 28.49      A   C
ATOM  1310  C   THR A 168     27.182  75.849  19.920  1.00 24.43      A   C
ATOM  1311  O   THR A 168     27.989  75.836  18.995  1.00 26.62      A   O
ATOM  1312  N   PRO A 169     27.347  76.640  20.992  1.00 25.87      A   N
ATOM  1313  CD  PRO A 169     26.337  76.983  22.009  1.00 23.89      A   C
ATOM  1314  CA  PRO A 169     28.512  77.523  21.113  1.00 28.42      A   C
ATOM  1315  CB  PRO A 169     28.198  78.329  22.372  1.00 25.95      A   C
ATOM  1316  CG  PRO A 169     26.709  78.406  22.351  1.00 26.22      A   C
ATOM  1317  C   PRO A 169     29.868  76.813  21.210  1.00 30.41      A   C
ATOM  1318  O   PRO A 169     30.914  77.440  21.035  1.00 30.45      A   O
ATOM  1319  N   LEU A 170     29.853  75.512  21.487  1.00 32.27      A   N
ATOM  1320  CA  LEU A 170     31.094  74.755  21.611  1.00 34.59      A   C
ATOM  1321  CB  LEU A 170     30.808  73.338  22.098  1.00 33.83      A   C
ATOM  1322  CG  LEU A 170     30.417  73.202  23.568  1.00 32.01      A   C
ATOM  1323  CD1 LEU A 170     30.035  71.760  23.848  1.00 29.69      A   C
ATOM  1324  CD2 LEU A 170     31.579  73.641  24.458  1.00 29.22      A   C
ATOM  1325  C   LEU A 170     31.897  74.677  20.323  1.00 37.74      A   C
ATOM  1326  O   LEU A 170     31.358  74.386  19.254  1.00 39.31      A   O
ATOM  1327  N   GLU A 171     33.197  74.924  20.434  1.00 40.03      A   N
ATOM  1328  CA  GLU A 171     34.076  74.871  19.276  1.00 43.34      A   C
ATOM  1329  CB  GLU A 171     34.750  76.229  19.067  1.00 48.27      A   C
ATOM  1330  CG  GLU A 171     33.759  77.349  18.782  1.00 54.56      A   C
ATOM  1331  CD  GLU A 171     33.072  77.200  17.431  1.00 59.45      A   C
ATOM  1332  OE1 GLU A 171     32.919  76.051  16.953  1.00 60.27      A   O
ATOM  1333  OE2 GLU A 171     32.672  78.237  16.852  1.00 61.77      A   O
ATOM  1334  C   GLU A 171     35.120  73.777  19.447  1.00 42.59      A   C
ATOM  1335  O   GLU A 171     36.239  73.888  18.951  1.00 43.77      A   O
ATOM  1336  N   ILE A 172     34.741  72.717  20.155  1.00 40.35      A   N
ATOM  1337  CA  ILE A 172     35.636  71.589  20.391  1.00 38.22      A   C
ATOM  1338  CB  ILE A 172     36.155  71.569  21.842  1.00 37.75      A   C
ATOM  1339  CG2 ILE A 172     36.806  72.901  22.184  1.00 34.13      A   C
ATOM  1340  CG1 ILE A 172     34.997  71.276  22.797  1.00 36.28      A   C
ATOM  1341  CD1 ILE A 172     35.430  70.993  24.225  1.00 40.90      A   C
ATOM  1342  C   ILE A 172     34.911  70.272  20.145  1.00 36.42      A   C
ATOM  1343  O   ILE A 172     33.688  70.200  20.222  1.00 39.20      A   O
ATOM  1344  N   LEU A 173     35.674  69.231  19.838  1.00 34.80      A   N
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Figure 6Y

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ATOM  1345  CA  LEU A 173      35.104  67.910  19.612  1.00 32.15      A   C
ATOM  1346  CB  LEU A 173      35.718  67.265  18.363  1.00 33.04      A   C
ATOM  1347  CG  LEU A 173      35.480  67.998  17.037  1.00 34.61      A   C
ATOM  1348  CD1 LEU A 173      36.221  67.290  15.910  1.00 33.74      A   C
ATOM  1349  CD2 LEU A 173      33.979  68.056  16.747  1.00 34.77      A   C
ATOM  1350  C   LEU A 173      35.454  67.102  20.855  1.00 29.45      A   C
ATOM  1351  O   LEU A 173      36.481  66.424  20.896  1.00 27.62      A   O
ATOM  1352  N   PRO A 174      34.598  67.167  21.891  1.00 27.18      A   N
ATOM  1353  CD  PRO A 174      33.272  67.811  21.931  1.00 26.43      A   C
ATOM  1354  CA  PRO A 174      34.858  66.432  23.132  1.00 24.33      A   C
ATOM  1355  CB  PRO A 174      33.646  66.772  24.003  1.00 25.04      A   C
ATOM  1356  CG  PRO A 174      32.560  67.015  22.997  1.00 27.39      A   C
ATOM  1357  C   PRO A 174      35.067  64.934  22.991  1.00 21.39      A   C
ATOM  1358  O   PRO A 174      34.335  64.250  22.277  1.00 22.17      A   O
ATOM  1359  N   GLU A 175      36.088  64.438  23.679  1.00 19.42      A   N
ATOM  1360  CA  GLU A 175      36.405  63.021  23.683  1.00 19.85      A   C
ATOM  1361  CB  GLU A 175      37.905  62.821  23.465  1.00 21.90      A   C
ATOM  1362  CG  GLU A 175      38.320  62.869  21.999  1.00 27.70      A   C
ATOM  1363  CD  GLU A 175      39.823  62.943  21.802  1.00 27.64      A   C
ATOM  1364  OE1 GLU A 175      40.565  62.242  22.523  1.00 28.19      A   O
ATOM  1365  OE2 GLU A 175      40.260  63.701  20.913  1.00 30.42      A   O
ATOM  1366  C   GLU A 175      35.983  62.473  25.044  1.00 19.80      A   C
ATOM  1367  O   GLU A 175      35.855  61.263  25.239  1.00 19.75      A   O
ATOM  1368  N   VAL A 176      35.762  63.383  25.986  1.00 18.80      A   N
ATOM  1369  CA  VAL A 176      35.349  63.006  27.330  1.00 17.58      A   C
ATOM  1370  CB  VAL A 176      36.550  62.981  28.313  1.00 16.92      A   C
ATOM  1371  CG1 VAL A 176      36.091  62.488  29.676  1.00 15.99      A   C
ATOM  1372  CG2 VAL A 176      37.661  62.087  27.772  1.00 16.67      A   C
ATOM  1373  C   VAL A 176      34.330  64.014  27.840  1.00 16.96      A   C
ATOM  1374  O   VAL A 176      34.533  65.224  27.746  1.00 17.95      A   O
ATOM  1375  N   ILE A 177      33.222  63.509  28.362  1.00 17.35      A   N
ATOM  1376  CA  ILE A 177      32.184  64.373  28.902  1.00 15.36      A   C
ATOM  1377  CB  ILE A 177      30.873  64.272  28.100  1.00 15.94      A   C
ATOM  1378  CG2 ILE A 177      29.805  65.149  28.759  1.00 14.07      A   C
ATOM  1379  CG1 ILE A 177      31.113  64.699  26.647  1.00 17.19      A   C
ATOM  1380  CD1 ILE A 177      29.880  64.597  25.748  1.00 18.12      A   C
ATOM  1381  C   ILE A 177      31.896  63.970  30.334  1.00 14.25      A   C
ATOM  1382  O   ILE A 177      31.499  62.833  30.609  1.00 15.75      A   O
ATOM  1383  N   ILE A 178      32.108  64.900  31.253  1.00 14.90      A   N
ATOM  1384  CA  ILE A 178      31.841  64.618  32.647  1.00 12.36      A   C
ATOM  1385  CB  ILE A 178      32.770  65.419  33.573  1.00 14.08      A   C
ATOM  1386  CG2 ILE A 178      32.465  65.085  35.026  1.00 10.97      A   C
ATOM  1387  CG1 ILE A 178      34.229  65.095  33.248  1.00 13.91      A   C
ATOM  1388  CD1 ILE A 178      35.235  65.846  34.106  1.00 13.08      A   C
ATOM  1389  C   ILE A 178      30.396  64.988  32.950  1.00 12.88      A   C
ATOM  1390  O   ILE A 178      29.949  66.103  32.671  1.00 13.50      A   O
ATOM  1391  N   LEU A 179      29.659  64.038  33.506  1.00 12.90      A   N
ATOM  1392  CA  LEU A 179      28.270  64.288  33.867  1.00 14.35      A   C
ATOM  1393  CB  LEU A 179      27.465  62.992  33.717  1.00 14.31      A   C
ATOM  1394  CG  LEU A 179      27.542  62.418  32.298  1.00 15.12      A   C
ATOM  1395  CD1 LEU A 179      26.919  61.033  32.251  1.00 20.10      A   C
ATOM  1396  CD2 LEU A 179      26.844  63.361  31.336  1.00 20.25      A   C
ATOM  1397  C   LEU A 179      28.320  64.760  35.319  1.00 13.67      A   C
ATOM  1398  O   LEU A 179      27.829  64.085  36.224  1.00 15.54      A   O
ATOM  1399  N   GLY A 180      28.930  65.931  35.512  1.00 11.65      A   N
ATOM  1400  CA  GLY A 180      29.117  66.517  36.834  1.00 12.90      A   C
ATOM  1401  C   GLY A 180      27.910  67.040  37.593  1.00 10.74      A   C
ATOM  1402  O   GLY A 180      27.955  68.116  38.191  1.00 12.43      A   O
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Figure 6Z

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ATOM  1403  N   CYS A 181     26.835  66.267  37.589  1.00 11.19      A   N
ATOM  1404  CA  CYS A 181     25.608  66.640  38.287  1.00 12.85      A   C
ATOM  1405  CB  CYS A 181     24.832  67.662  37.455  1.00 10.63      A   C
ATOM  1406  SG  CYS A 181     23.232  68.156  38.139  1.00 12.80      A   S
ATOM  1407  C   CYS A 181     24.769  65.379  38.482  1.00 10.40      A   C
ATOM  1408  O   CYS A 181     24.655  64.567  37.565  1.00 12.33      A   O
ATOM  1409  N   THR A 182     24.195  65.218  39.673  1.00 11.84      A   N
ATOM  1410  CA  THR A 182     23.374  64.050  39.993  1.00 10.35      A   C
ATOM  1411  CB  THR A 182     22.661  64.207  41.363  1.00 10.67      A   C
ATOM  1412  OG1 THR A 182     21.912  65.435  41.381  1.00  8.58      A   O
ATOM  1413  CG2 THR A 182     23.672  64.197  42.500  1.00  7.64      A   C
ATOM  1414  C   THR A 182     22.283  63.760  38.966  1.00 11.06      A   C
ATOM  1415  O   THR A 182     21.936  62.610  38.733  1.00 10.76      A   O
ATOM  1416  N   HIS A 183     21.739  64.810  38.364  1.00  9.82      A   N
ATOM  1417  CA  HIS A 183     20.649  64.666  37.400  1.00 12.23      A   C
ATOM  1418  CB  HIS A 183     19.884  65.990  37.276  1.00 10.20      A   C
ATOM  1419  CG  HIS A 183     19.136  66.386  38.510  1.00 10.97      A   C
ATOM  1420  CD2 HIS A 183     17.905  66.930  38.668  1.00  7.50      A   C
ATOM  1421  ND1 HIS A 183     19.677  66.290  39.774  1.00 11.77      A   N
ATOM  1422  CE1 HIS A 183     18.812  66.758  40.658  1.00 10.61      A   C
ATOM  1423  NE2 HIS A 183     17.729  67.154  40.012  1.00 10.59      A   N
ATOM  1424  C   HIS A 183     21.020  64.221  35.990  1.00 10.73      A   C
ATOM  1425  O   HIS A 183     20.228  63.569  35.323  1.00 12.38      A   O
ATOM  1426  N   PHE A 184     22.221  64.570  35.545  1.00 12.86      A   N
ATOM  1427  CA  PHE A 184     22.645  64.280  34.180  1.00 12.13      A   C
ATOM  1428  CB  PHE A 184     23.988  64.976  33.925  1.00 11.91      A   C
ATOM  1429  CG  PHE A 184     23.927  66.488  34.096  1.00 11.77      A   C
ATOM  1430  CD1 PHE A 184     25.057  67.276  33.896  1.00 13.67      A   C
ATOM  1431  CD2 PHE A 184     22.739  67.116  34.482  1.00  9.45      A   C
ATOM  1432  CE1 PHE A 184     25.009  68.666  34.081  1.00 11.33      A   C
ATOM  1433  CE2 PHE A 184     22.681  68.502  34.670  1.00 12.83      A   C
ATOM  1434  CZ  PHE A 184     23.819  69.278  34.469  1.00  9.95      A   C
ATOM  1435  C   PHE A 184     22.655  62.833  33.670  1.00 12.53      A   C
ATOM  1436  O   PHE A 184     22.429  62.596  32.481  1.00 14.09      A   O
ATOM  1437  N   PRO A 185     22.902  61.847  34.545  1.00 13.81      A   N
ATOM  1438  CD  PRO A 185     23.442  61.881  35.918  1.00 14.48      A   C
ATOM  1439  CA  PRO A 185     22.893  60.475  34.026  1.00 13.96      A   C
ATOM  1440  CB  PRO A 185     23.165  59.640  35.275  1.00 14.58      A   C
ATOM  1441  CG  PRO A 185     24.112  60.522  36.032  1.00 12.13      A   C
ATOM  1442  C   PRO A 185     21.554  60.121  33.367  1.00 15.04      A   C
ATOM  1443  O   PRO A 185     21.492  59.261  32.489  1.00 13.75      A   O
ATOM  1444  N   LEU A 186     20.485  60.790  33.791  1.00 13.98      A   N
ATOM  1445  CA  LEU A 186     19.156  60.525  33.243  1.00 13.19      A   C
ATOM  1446  CB  LEU A 186     18.080  61.193  34.108  1.00 13.71      A   C
ATOM  1447  CG  LEU A 186     17.634  60.379  35.334  1.00 15.55      A   C
ATOM  1448  CD1 LEU A 186     18.802  60.174  36.288  1.00 18.92      A   C
ATOM  1449  CD2 LEU A 186     16.493  61.099  36.027  1.00 14.26      A   C
ATOM  1450  C   LEU A 186     18.982  60.931  31.778  1.00 14.41      A   C
ATOM  1451  O   LEU A 186     18.010  60.533  31.137  1.00 14.59      A   O
ATOM  1452  N   ILE A 187     19.905  61.734  31.255  1.00 14.30      A   N
ATOM  1453  CA  ILE A 187     19.854  62.140  29.849  1.00 14.33      A   C
ATOM  1454  CB  ILE A 187     19.485  63.633  29.667  1.00 13.17      A   C
ATOM  1455  CG2 ILE A 187     18.052  63.871  30.096  1.00 11.03      A   C
ATOM  1456  CG1 ILE A 187     20.446  64.523  30.453  1.00 12.17      A   C
ATOM  1457  CD1 ILE A 187     20.256  66.011  30.170  1.00 14.07      A   C
ATOM  1458  C   ILE A 187     21.197  61.890  29.168  1.00 14.64      A   C
ATOM  1459  O   ILE A 187     21.487  62.447  28.108  1.00 13.68      A   O
ATOM  1460  N   ALA A 188     22.008  61.035  29.781  1.00 15.37      A   N
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Figure 6AA

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ATOM  1461  CA  ALA A 188      23.322  60.707  29.243  1.00 16.86      A   C
ATOM  1462  CB  ALA A 188      23.965  59.607  30.075  1.00 15.17      A   C
ATOM  1463  C   ALA A 188      23.244  60.280  27.776  1.00 17.17      A   C
ATOM  1464  O   ALA A 188      23.979  60.797  26.938  1.00 15.74      A   O
ATOM  1465  N   GLN A 189      22.353  59.340  27.470  1.00 17.32      A   N
ATOM  1466  CA  GLN A 189      22.203  58.857  26.101  1.00 18.82      A   C
ATOM  1467  CB  GLN A 189      21.162  57.741  26.050  1.00 23.61      A   C
ATOM  1468  CG  GLN A 189      21.199  56.919  24.774  1.00 30.80      A   C
ATOM  1469  CD  GLN A 189      22.592  56.391  24.458  1.00 36.03      A   C
ATOM  1470  OE1 GLN A 189      23.321  55.942  25.347  1.00 36.39      A   O
ATOM  1471  NE2 GLN A 189      22.965  56.435  23.184  1.00 38.93      A   N
ATOM  1472  C   GLN A 189      21.794  59.995  25.169  1.00 17.49      A   C
ATOM  1473  O   GLN A 189      22.280  60.092  24.041  1.00 17.22      A   O
ATOM  1474  N   LYS A 190      20.894  60.851  25.639  1.00 17.64      A   N
ATOM  1475  CA  LYS A 190      20.449  61.986  24.841  1.00 16.93      A   C
ATOM  1476  CB  LYS A 190      19.338  62.750  25.565  1.00 17.51      A   C
ATOM  1477  CG  LYS A 190      17.998  62.038  25.578  1.00 21.98      A   C
ATOM  1478  CD  LYS A 190      17.462  61.852  24.166  1.00 25.56      A   C
ATOM  1479  CE  LYS A 190      16.064  61.256  24.188  1.00 30.02      A   C
ATOM  1480  NZ  LYS A 190      15.428  61.242  22.839  1.00 32.59      A   N
ATOM  1481  C   LYS A 190      21.624  62.919  24.572  1.00 17.12      A   C
ATOM  1482  O   LYS A 190      21.755  63.468  23.481  1.00 19.51      A   O
ATOM  1483  N   ILE A 191      22.483  63.097  25.570  1.00 15.92      A   N
ATOM  1484  CA  ILE A 191      23.643  63.963  25.413  1.00 15.53      A   C
ATOM  1485  CB  ILE A 191      24.348  64.194  26.769  1.00 16.74      A   C
ATOM  1486  CG2 ILE A 191      25.698  64.877  26.558  1.00 17.54      A   C
ATOM  1487  CG1 ILE A 191      23.447  65.048  27.668  1.00 16.67      A   C
ATOM  1488  CD1 ILE A 191      24.051  65.372  29.014  1.00 17.95      A   C
ATOM  1489  C   ILE A 191      24.615  63.350  24.413  1.00 17.26      A   C
ATOM  1490  O   ILE A 191      25.099  64.027  23.508  1.00 16.51      A   O
ATOM  1491  N   GLU A 192      24.892  62.062  24.566  1.00 17.44      A   N
ATOM  1492  CA  GLU A 192      25.792  61.387  23.643  1.00 18.42      A   C
ATOM  1493  CB  GLU A 192      25.937  59.909  24.007  1.00 20.11      A   C
ATOM  1494  CG  GLU A 192      26.885  59.159  23.085  1.00 26.76      A   C
ATOM  1495  CD  GLU A 192      26.872  57.665  23.322  1.00 32.66      A   C
ATOM  1496  OE1 GLU A 192      25.884  57.005  22.936  1.00 37.07      A   O
ATOM  1497  OE2 GLU A 192      27.846  57.152  23.906  1.00 37.14      A   O
ATOM  1498  C   GLU A 192      25.209  61.499  22.241  1.00 17.46      A   C
ATOM  1499  O   GLU A 192      25.912  61.804  21.283  1.00 15.49      A   O
ATOM  1500  N   GLY A 193      23.910  61.249  22.136  1.00 19.60      A   N
ATOM  1501  CA  GLY A 193      23.247  61.319  20.851  1.00 18.22      A   C
ATOM  1502  C   GLY A 193      23.344  62.683  20.199  1.00 20.98      A   C
ATOM  1503  O   GLY A 193      23.518  62.781  18.983  1.00 19.02      A   O
ATOM  1504  N   TYR A 194      23.230  63.742  20.997  1.00 19.99      A   N
ATOM  1505  CA  TYR A 194      23.302  65.087  20.450  1.00 19.30      A   C
ATOM  1506  CB  TYR A 194      23.081  66.136  21.545  1.00 21.79      A   C
ATOM  1507  CG  TYR A 194      23.038  67.544  20.997  1.00 22.73      A   C
ATOM  1508  CD1 TYR A 194      21.822  68.170  20.713  1.00 25.33      A   C
ATOM  1509  CE1 TYR A 194      21.784  69.442  20.133  1.00 26.15      A   C
ATOM  1510  CD2 TYR A 194      24.216  68.226  20.692  1.00 24.23      A   C
ATOM  1511  CE2 TYR A 194      24.190  69.493  20.109  1.00 23.26      A   C
ATOM  1512  CZ  TYR A 194      22.973  70.092  19.830  1.00 25.26      A   C
ATOM  1513  OH  TYR A 194      22.941  71.327  19.222  1.00 28.86      A   O
ATOM  1514  C   TYR A 194      24.660  65.313  19.788  1.00 20.71      A   C
ATOM  1515  O   TYR A 194      24.738  65.782  18.653  1.00 18.94      A   O
ATOM  1516  N   PHE A 195      25.732  64.980  20.496  1.00 19.26      A   N
ATOM  1517  CA  PHE A 195      27.062  65.169  19.942  1.00 21.38      A   C
ATOM  1518  CB  PHE A 195      28.126  64.952  21.020  1.00 20.73      A   C
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Figure 6BB

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ATOM  1519  CG  PHE A 195     28.251  66.103  21.971  1.00 20.61      A   C
ATOM  1520  CD1 PHE A 195     27.488  66.158  23.131  1.00 19.23      A   C
ATOM  1521  CD2 PHE A 195     29.097  67.165  21.673  1.00 21.43      A   C
ATOM  1522  CE1 PHE A 195     27.565  67.263  23.986  1.00 20.28      A   C
ATOM  1523  CE2 PHE A 195     29.183  68.273  22.515  1.00 18.52      A   C
ATOM  1524  CZ  PHE A 195     28.416  68.323  23.673  1.00 19.62      A   C
ATOM  1525  C   PHE A 195     27.352  64.290  18.730  1.00 21.31      A   C
ATOM  1526  O   PHE A 195     28.045  64.713  17.806  1.00 21.45      A   O
ATOM  1527  N   MET A 196     26.822  63.072  18.720  1.00 22.22      A   N
ATOM  1528  CA  MET A 196     27.059  62.190  17.584  1.00 24.31      A   C
ATOM  1529  CB  MET A 196     26.655  60.749  17.915  1.00 25.67      A   C
ATOM  1530  CG  MET A 196     27.528  60.084  18.971  1.00 26.49      A   C
ATOM  1531  SD  MET A 196     29.295  60.205  18.575  1.00 30.70      A   S
ATOM  1532  CE  MET A 196     29.481  58.865  17.401  1.00 31.02      A   C
ATOM  1533  C   MET A 196     26.293  62.667  16.354  1.00 25.42      A   C
ATOM  1534  O   MET A 196     26.734  62.451  15.227  1.00 23.73      A   O
ATOM  1535  N   GLY A 197     25.157  63.328  16.571  1.00 25.90      A   N
ATOM  1536  CA  GLY A 197     24.361  63.805  15.451  1.00 26.44      A   C
ATOM  1537  C   GLY A 197     24.566  65.258  15.054  1.00 29.06      A   C
ATOM  1538  O   GLY A 197     24.129  65.681  13.981  1.00 30.51      A   O
ATOM  1539  N   HIS A 198     25.233  66.030  15.903  1.00 27.75      A   N
ATOM  1540  CA  HIS A 198     25.456  67.441  15.612  1.00 28.55      A   C
ATOM  1541  CB  HIS A 198     24.824  68.293  16.705  1.00 28.88      A   C
ATOM  1542  CG  HIS A 198     23.330  68.234  16.718  1.00 26.12      A   C
ATOM  1543  CD2 HIS A 198     22.470  67.535  17.495  1.00 26.28      A   C
ATOM  1544  ND1 HIS A 198     22.553  68.943  15.828  1.00 27.58      A   N
ATOM  1545  CE1 HIS A 198     21.277  68.687  16.060  1.00 27.01      A   C
ATOM  1546  NE2 HIS A 198     21.200  67.835  17.066  1.00 26.83      A   N
ATOM  1547  C   HIS A 198     26.923  67.792  15.457  1.00 30.79      A   C
ATOM  1548  O   HIS A 198     27.270  68.941  15.180  1.00 32.29      A   O
ATOM  1549  N   PHE A 199     27.785  66.800  15.644  1.00 30.80      A   N
ATOM  1550  CA  PHE A 199     29.220  66.999  15.498  1.00 33.66      A   C
ATOM  1551  CB  PHE A 199     29.906  67.052  16.866  1.00 35.46      A   C
ATOM  1552  CG  PHE A 199     29.565  68.275  17.676  1.00 39.04      A   C
ATOM  1553  CD1 PHE A 199     28.281  68.463  18.182  1.00 39.24      A   C
ATOM  1554  CD2 PHE A 199     30.537  69.237  17.945  1.00 40.88      A   C
ATOM  1555  CE1 PHE A 199     27.968  69.591  18.944  1.00 40.57      A   C
ATOM  1556  CE2 PHE A 199     30.236  70.370  18.707  1.00 42.99      A   C
ATOM  1557  CZ  PHE A 199     28.948  70.547  19.207  1.00 40.25      A   C
ATOM  1558  C   PHE A 199     29.790  65.855  14.673  1.00 32.87      A   C
ATOM  1559  O   PHE A 199     29.170  64.798  14.547  1.00 32.00      A   O
ATOM  1560  N   ALA A 200     30.972  66.064  14.108  1.00 34.09      A   N
ATOM  1561  CA  ALA A 200     31.605  65.040  13.288  1.00 34.34      A   C
ATOM  1562  CB  ALA A 200     32.381  65.690  12.154  1.00 35.22      A   C
ATOM  1563  C   ALA A 200     32.532  64.168  14.119  1.00 34.93      A   C
ATOM  1564  O   ALA A 200     33.704  63.996  13.782  1.00 35.08      A   O
ATOM  1565  N   LEU A 201     32.012  63.618  15.209  1.00 34.85      A   N
ATOM  1566  CA  LEU A 201     32.821  62.765  16.067  1.00 34.78      A   C
ATOM  1567  CB  LEU A 201     32.210  62.690  17.472  1.00 35.79      A   C
ATOM  1568  CG  LEU A 201     32.120  64.015  18.231  1.00 35.31      A   C
ATOM  1569  CD1 LEU A 201     31.513  63.760  19.603  1.00 35.13      A   C
ATOM  1570  CD2 LEU A 201     33.498  64.641  18.365  1.00 35.35      A   C
ATOM  1571  C   LEU A 201     32.906  61.366  15.462  1.00 34.07      A   C
ATOM  1572  O   LEU A 201     31.887  60.773  15.104  1.00 35.38      A   O
ATOM  1573  N   PRO A 202     34.128  60.817  15.344  1.00 33.66      A   N
ATOM  1574  CD  PRO A 202     35.409  61.457  15.698  1.00 32.39      A   C
ATOM  1575  CA  PRO A 202     34.353  59.475  14.779  1.00 32.85      A   C
ATOM  1576  CB  PRO A 202     35.872  59.404  14.655  1.00 33.65      A   C
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Figure 6CC

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ATOM  1577  CG  PRO A 202      36.343  60.272  15.793  1.00 34.48      A   C
ATOM  1578  C   PRO A 202      33.790  58.355  15.649  1.00 33.17      A   C
ATOM  1579  O   PRO A 202      33.402  57.297  15.151  1.00 30.49      A   O
ATOM  1580  N   THR A 203      33.773  58.599  16.956  1.00 31.52      A   N
ATOM  1581  CA  THR A 203      33.248  57.634  17.919  1.00 31.65      A   C
ATOM  1582  CB  THR A 203      34.338  56.676  18.426  1.00 32.68      A   C
ATOM  1583  OG1 THR A 203      35.425  57.424  18.979  1.00 35.29      A   O
ATOM  1584  CG2 THR A 203      34.828  55.781  17.302  1.00 37.32      A   C
ATOM  1585  C   THR A 203      32.688  58.386  19.117  1.00 30.86      A   C
ATOM  1586  O   THR A 203      33.168  59.451  19.461  1.00 27.18      A   O
ATOM  1587  N   PRO A 204      31.671  57.817  19.775  1.00 29.89      A   N
ATOM  1588  CD  PRO A 204      31.126  56.473  19.492  1.00 29.77      A   C
ATOM  1589  CA  PRO A 204      31.061  58.463  20.945  1.00 28.24      A   C
ATOM  1590  CB  PRO A 204      30.047  57.449  21.462  1.00 29.94      A   C
ATOM  1591  CG  PRO A 204      30.111  56.276  20.568  1.00 30.77      A   C
ATOM  1592  C   PRO A 204      32.096  58.803  22.007  1.00 25.79      A   C
ATOM  1593  O   PRO A 204      33.032  58.041  22.269  1.00 25.89      A   O
ATOM  1594  N   PRO A 205      31.961  59.981  22.626  1.00 23.44      A   N
ATOM  1595  CD  PRO A 205      30.990  61.063  22.358  1.00 24.13      A   C
ATOM  1596  CA  PRO A 205      32.915  60.378  23.670  1.00 22.08      A   C
ATOM  1597  CB  PRO A 205      32.600  61.852  23.873  1.00 24.52      A   C
ATOM  1598  CG  PRO A 205      31.125  61.932  23.587  1.00 24.69      A   C
ATOM  1599  C   PRO A 205      32.705  59.546  24.927  1.00 19.36      A   C
ATOM  1600  O   PRO A 205      31.637  58.961  25.125  1.00 18.49      A   O
ATOM  1601  N   LEU A 206      33.722  59.492  25.776  1.00 18.43      A   N
ATOM  1602  CA  LEU A 206      33.626  58.762  27.037  1.00 18.50      A   C
ATOM  1603  CB  LEU A 206      35.018  58.513  27.619  1.00 20.51      A   C
ATOM  1604  CG  LEU A 206      35.095  57.847  28.996  1.00 22.39      A   C
ATOM  1605  CD1 LEU A 206      34.491  56.439  28.946  1.00 22.36      A   C
ATOM  1606  CD2 LEU A 206      36.552  57.791  29.435  1.00 24.60      A   C
ATOM  1607  C   LEU A 206      32.822  59.615  28.017  1.00 18.04      A   C
ATOM  1608  O   LEU A 206      33.163  60.770  28.253  1.00 16.95      A   O
ATOM  1609  N   LEU A 207      31.746  59.049  28.554  1.00 16.00      A   N
ATOM  1610  CA  LEU A 207      30.909  59.748  29.521  1.00 17.26      A   C
ATOM  1611  CB  LEU A 207      29.433  59.412  29.304  1.00 18.06      A   C
ATOM  1612  CG  LEU A 207      28.664  60.071  28.158  1.00 24.42      A   C
ATOM  1613  CD1 LEU A 207      29.448  59.984  26.863  1.00 25.51      A   C
ATOM  1614  CD2 LEU A 207      27.310  59.373  28.012  1.00 24.48      A   C
ATOM  1615  C   LEU A 207      31.318  59.314  30.922  1.00 16.98      A   C
ATOM  1616  O   LEU A 207      31.388  58.120  31.215  1.00 18.46      A   O
ATOM  1617  N   ILE A 208      31.592  60.276  31.792  1.00 13.50      A   N
ATOM  1618  CA  ILE A 208      31.983  59.940  33.150  1.00 14.98      A   C
ATOM  1619  CB  ILE A 208      33.112  60.864  33.659  1.00 16.20      A   C
ATOM  1620  CG2 ILE A 208      33.468  60.509  35.101  1.00 16.97      A   C
ATOM  1621  CG1 ILE A 208      34.345  60.722  32.763  1.00 16.39      A   C
ATOM  1622  CD1 ILE A 208      34.984  59.333  32.784  1.00 17.91      A   C
ATOM  1623  C   ILE A 208      30.771  60.069  34.057  1.00 15.79      A   C
ATOM  1624  O   ILE A 208      30.193  61.150  34.194  1.00 15.47      A   O
ATOM  1625  N   HIS A 209      30.390  58.951  34.669  1.00 15.02      A   N
ATOM  1626  CA  HIS A 209      29.238  58.895  35.567  1.00 14.90      A   C
ATOM  1627  CB  HIS A 209      28.502  57.569  35.333  1.00 17.49      A   C
ATOM  1628  CG  HIS A 209      27.271  57.387  36.169  1.00 19.71      A   C
ATOM  1629  CD2 HIS A 209      27.116  57.192  37.500  1.00 20.19      A   C
ATOM  1630  ND1 HIS A 209      26.004  57.336  35.625  1.00 21.72      A   N
ATOM  1631  CE1 HIS A 209      25.123  57.114  36.584  1.00 17.63      A   C
ATOM  1632  NE2 HIS A 209      25.772  57.023  37.732  1.00 22.48      A   N
ATOM  1633  C   HIS A 209      29.744  59.006  37.011  1.00 13.24      A   C
ATOM  1634  O   HIS A 209      30.546  58.191  37.458  1.00 13.01      A   O
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Figure 6DD

ATOM 1635 N SER A 210 29.275 60.018 37.734 1.00 12.05 A N
ATOM 1636 CA SER A 210 29.709 60.238 39.109 1.00 11.23 A C
ATOM 1637 CB SER A 210 28.977 61.442 39.701 1.00 11.83 A C
ATOM 1638 OG SER A 210 29.140 62.587 38.881 1.00 12.14 A O
ATOM 1639 C SER A 210 29.529 59.031 40.032 1.00 12.17 A C
ATOM 1640 O SER A 210 30.370 58.774 40.890 1.00 11.45 A O
ATOM 1641 N GLY A 211 28.432 58.303 39.861 1.00 13.88 A N
ATOM 1642 CA GLY A 211 28.178 57.142 40.698 1.00 15.08 A C
ATOM 1643 C GLY A 211 29.147 56.004 40.446 1.00 16.38 A C
ATOM 1644 O GLY A 211 29.744 55.461 41.378 1.00 15.04 A O
ATOM 1645 N ASP A 212 29.311 55.630 39.183 1.00 15.98 A N
ATOM 1646 CA ASP A 212 30.231 54.552 38.860 1.00 16.82 A C
ATOM 1647 CB ASP A 212 30.208 54.264 37.365 1.00 19.63 A C
ATOM 1648 CG ASP A 212 28.847 53.798 36.895 1.00 23.61 A C
ATOM 1649 OD1 ASP A 212 28.145 53.131 37.692 1.00 25.34 A O
ATOM 1650 OD2 ASP A 212 28.486 54.086 35.738 1.00 21.50 A O
ATOM 1651 C ASP A 212 31.638 54.917 39.303 1.00 16.04 A C
ATOM 1652 O ASP A 212 32.375 54.073 39.807 1.00 15.40 A O
ATOM 1653 N ALA A 213 31.994 56.185 39.135 1.00 12.67 A N
ATOM 1654 CA ALA A 213 33.317 56.667 39.517 1.00 14.11 A C
ATOM 1655 CB ALA A 213 33.493 58.126 39.076 1.00 11.29 A C
ATOM 1656 C ALA A 213 33.560 56.540 41.022 1.00 12.53 A C
ATOM 1657 O ALA A 213 34.607 56.049 41.452 1.00 13.00 A O
ATOM 1658 N ILE A 214 32.603 56.973 41.834 1.00 13.61 A N
ATOM 1659 CA ILE A 214 32.808 56.875 43.271 1.00 11.94 A C
ATOM 1660 CB ILE A 214 31.748 57.701 44.065 1.00 12.63 A C
ATOM 1661 CG2 ILE A 214 30.367 57.085 43.938 1.00 15.04 A C
ATOM 1662 CG1 ILE A 214 32.174 57.795 45.530 1.00 12.30 A C
ATOM 1663 CD1 ILE A 214 31.429 58.832 46.317 1.00 11.04 A C
ATOM 1664 C ILE A 214 32.855 55.405 43.719 1.00 13.71 A C
ATOM 1665 O ILE A 214 33.595 55.061 44.643 1.00 12.81 A O
ATOM 1666 N VAL A 215 32.096 54.538 43.053 1.00 13.33 A N
ATOM 1667 CA VAL A 215 32.118 53.109 43.387 1.00 13.18 A C
ATOM 1668 CB VAL A 215 31.165 52.293 42.474 1.00 13.68 A C
ATOM 1669 CG1 VAL A 215 31.481 50.792 42.579 1.00 14.80 A C
ATOM 1670 CG2 VAL A 215 29.707 52.537 42.876 1.00 10.93 A C
ATOM 1671 C VAL A 215 33.550 52.599 43.190 1.00 15.07 A C
ATOM 1672 O VAL A 215 34.115 51.933 44.065 1.00 12.73 A O
ATOM 1673 N GLU A 216 34.136 52.924 42.039 1.00 13.86 A N
ATOM 1674 CA GLU A 216 35.503 52.511 41.738 1.00 17.89 A C
ATOM 1675 CB GLU A 216 35.973 53.120 40.414 1.00 21.27 A C
ATOM 1676 CG GLU A 216 35.112 52.807 39.204 1.00 27.92 A C
ATOM 1677 CD GLU A 216 35.637 53.492 37.941 1.00 34.02 A C
ATOM 1678 OE1 GLU A 216 36.824 53.286 37.609 1.00 31.93 A O
ATOM 1679 OE2 GLU A 216 34.868 54.236 37.285 1.00 35.33 A O
ATOM 1680 C GLU A 216 36.447 52.971 42.846 1.00 17.32 A C
ATOM 1681 O GLU A 216 37.245 52.188 43.363 1.00 16.80 A O
ATOM 1682 N TYR A 217 36.352 54.248 43.204 1.00 16.20 A N
ATOM 1683 CA TYR A 217 37.200 54.818 44.244 1.00 16.23 A C
ATOM 1684 CB TYR A 217 36.900 56.308 44.432 1.00 14.73 A C
ATOM 1685 CG TYR A 217 37.693 56.942 45.557 1.00 17.55 A C
ATOM 1686 CD1 TYR A 217 39.053 57.202 45.418 1.00 18.17 A C
ATOM 1687 CE1 TYR A 217 39.797 57.738 46.475 1.00 18.51 A C
ATOM 1688 CD2 TYR A 217 37.089 57.234 46.780 1.00 16.61 A C
ATOM 1689 CE2 TYR A 217 37.815 57.765 47.836 1.00 17.74 A C
ATOM 1690 CZ TYR A 217 39.168 58.014 47.680 1.00 19.47 A C
ATOM 1691 OH TYR A 217 39.891 58.526 48.735 1.00 18.42 A O
ATOM 1692 C TYR A 217 37.041 54.116 45.584 1.00 16.31 A C

Figure 6EE

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ATOM  1693  O   TYR A 217     38.028  53.715  46.199  1.00 16.78      A   O
ATOM  1694  N   LEU A 218     35.798  53.995  46.045  1.00 15.56      A   N
ATOM  1695  CA  LEU A 218     35.509  53.353  47.324  1.00 18.16      A   C
ATOM  1696  CB  LEU A 218     33.993  53.344  47.575  1.00 15.21      A   C
ATOM  1697  CG  LEU A 218     33.321  54.705  47.799  1.00 15.27      A   C
ATOM  1698  CD1 LEU A 218     31.798  54.546  47.756  1.00 14.34      A   C
ATOM  1699  CD2 LEU A 218     33.775  55.294  49.129  1.00 13.25      A   C
ATOM  1700  C   LEU A 218     36.058  51.926  47.402  1.00 18.45      A   C
ATOM  1701  O   LEU A 218     36.648  51.531  48.409  1.00 18.06      A   O
ATOM  1702  N   GLN A 219     35.871  51.150  46.341  1.00 17.77      A   N
ATOM  1703  CA  GLN A 219     36.367  49.778  46.335  1.00 19.66      A   C
ATOM  1704  CB  GLN A 219     36.042  49.097  45.005  1.00 18.42      A   C
ATOM  1705  CG  GLN A 219     34.577  49.147  44.645  1.00 17.80      A   C
ATOM  1706  CD  GLN A 219     34.282  48.496  43.318  1.00 17.89      A   C
ATOM  1707  OE1 GLN A 219     35.071  48.596  42.372  1.00 18.96      A   O
ATOM  1708  NE2 GLN A 219     33.134  47.837  43.228  1.00 13.87      A   N
ATOM  1709  C   GLN A 219     37.876  49.740  46.567  1.00 19.63      A   C
ATOM  1710  O   GLN A 219     38.368  48.964  47.380  1.00 19.95      A   O
ATOM  1711  N   GLN A 220     38.605  50.593  45.859  1.00 21.16      A   N
ATOM  1712  CA  GLN A 220     40.057  50.621  45.992  1.00 24.11      A   C
ATOM  1713  CB  GLN A 220     40.681  51.372  44.811  1.00 25.85      A   C
ATOM  1714  CG  GLN A 220     42.197  51.445  44.885  1.00 34.94      A   C
ATOM  1715  CD  GLN A 220     42.830  51.975  43.615  1.00 40.03      A   C
ATOM  1716  OE1 GLN A 220     44.050  52.152  43.548  1.00 44.37      A   O
ATOM  1717  NE2 GLN A 220     42.010  52.227  42.598  1.00 41.95      A   N
ATOM  1718  C   GLN A 220     40.534  51.242  47.304  1.00 22.63      A   C
ATOM  1719  O   GLN A 220     41.275  50.617  48.062  1.00 21.00      A   O
ATOM  1720  N   LYS A 221     40.104  52.472  47.564  1.00 21.71      A   N
ATOM  1721  CA  LYS A 221     40.503  53.194  48.770  1.00 22.37      A   C
ATOM  1722  CB  LYS A 221     39.830  54.570  48.795  1.00 21.53      A   C
ATOM  1723  CG  LYS A 221     39.984  55.325  50.111  1.00 25.31      A   C
ATOM  1724  CD  LYS A 221     41.443  55.615  50.439  1.00 26.19      A   C
ATOM  1725  CE  LYS A 221     41.579  56.244  51.818  1.00 29.00      A   C
ATOM  1726  NZ  LYS A 221     42.999  56.511  52.159  1.00 29.71      A   N
ATOM  1727  C   LYS A 221     40.221  52.464  50.084  1.00 22.42      A   C
ATOM  1728  O   LYS A 221     41.090  52.376  50.953  1.00 21.37      A   O
ATOM  1729  N   TYR A 222     39.005  51.950  50.229  1.00 20.94      A   N
ATOM  1730  CA  TYR A 222     38.616  51.250  51.442  1.00 21.75      A   C
ATOM  1731  CB  TYR A 222     37.251  51.762  51.903  1.00 22.02      A   C
ATOM  1732  CG  TYR A 222     37.277  53.247  52.204  1.00 20.42      A   C
ATOM  1733  CD1 TYR A 222     36.737  54.178  51.314  1.00 18.91      A   C
ATOM  1734  CE1 TYR A 222     36.866  55.549  51.545  1.00 20.88      A   C
ATOM  1735  CD2 TYR A 222     37.938  53.725  53.336  1.00 21.77      A   C
ATOM  1736  CE2 TYR A 222     38.074  55.080  53.577  1.00 19.97      A   C
ATOM  1737  CZ  TYR A 222     37.540  55.988  52.679  1.00 20.71      A   C
ATOM  1738  OH  TYR A 222     37.705  57.330  52.909  1.00 16.95      A   O
ATOM  1739  C   TYR A 222     38.637  49.731  51.350  1.00 21.67      A   C
ATOM  1740  O   TYR A 222     38.112  49.040  52.226  1.00 20.83      A   O
ATOM  1741  N   ALA A 223     39.264  49.219  50.292  1.00 21.20      A   N
ATOM  1742  CA  ALA A 223     39.408  47.774  50.077  1.00 22.92      A   C
ATOM  1743  CB  ALA A 223     40.466  47.204  50.984  1.00 23.23      A   C
ATOM  1744  C   ALA A 223     38.105  47.055  50.330  1.00 23.19      A   C
ATOM  1745  O   ALA A 223     38.024  46.162  51.180  1.00 20.95      A   O
ATOM  1746  N   LEU A 224     37.088  47.426  49.565  1.00 25.19      A   N
ATOM  1747  CA  LEU A 224     35.759  46.839  49.692  1.00 24.53      A   C
ATOM  1748  CB  LEU A 224     34.703  47.937  49.609  1.00 22.99      A   C
ATOM  1749  CG  LEU A 224     34.869  49.090  50.607  1.00 21.68      A   C
ATOM  1750  CD1 LEU A 224     33.731  50.099  50.443  1.00 22.66      A   C
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Figure 6FF

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ATOM  1751  CD2 LEU A 224     34.875  48.531  52.022  1.00 23.83    A   C
ATOM  1752  C   LEU A 224     35.576  45.852  48.551  1.00 24.10    A   C
ATOM  1753  O   LEU A 224     35.569  46.259  47.400  1.00 22.11    A   O
ATOM  1754  N   LYS A 225     35.368  44.572  48.866  1.00 26.47    A   N
ATOM  1755  CA  LYS A 225     35.212  43.532  47.846  1.00 25.75    A   C
ATOM  1756  CB  LYS A 225     35.880  42.233  48.331  1.00 26.74    A   C
ATOM  1757  CG  LYS A 225     37.358  42.380  48.669  1.00 28.32    A   C
ATOM  1758  CD  LYS A 225     38.185  42.652  47.421  1.00 31.42    A   C
ATOM  1759  CE  LYS A 225     38.157  41.461  46.478  1.00 32.69    A   C
ATOM  1760  NZ  LYS A 225     39.003  41.698  45.284  1.00 34.46    A   N
ATOM  1761  C   LYS A 225     33.803  43.213  47.340  1.00 24.95    A   C
ATOM  1762  O   LYS A 225     33.568  42.125  46.819  1.00 29.54    A   O
ATOM  1763  N   ASN A 226     32.870  44.143  47.489  1.00 23.13    A   N
ATOM  1764  CA  ASN A 226     31.498  43.938  47.019  1.00 20.01    A   C
ATOM  1765  CB  ASN A 226     31.469  43.729  45.500  1.00 19.42    A   C
ATOM  1766  CG  ASN A 226     32.287  44.755  44.751  1.00 23.12    A   C
ATOM  1767  OD1 ASN A 226     33.342  44.439  44.190  1.00 20.38    A   O
ATOM  1768  ND2 ASN A 226     31.814  45.995  44.743  1.00 16.65    A   N
ATOM  1769  C   ASN A 226     30.800  42.740  47.662  1.00 21.21    A   C
ATOM  1770  O   ASN A 226     30.086  41.999  46.981  1.00 18.29    A   O
ATOM  1771  N   ASN A 227     30.984  42.551  48.963  1.00 22.29    A   N
ATOM  1772  CA  ASN A 227     30.362  41.421  49.641  1.00 22.96    A   C
ATOM  1773  CB  ASN A 227     31.438  40.462  50.163  1.00 22.46    A   C
ATOM  1774  CG  ASN A 227     32.503  41.165  50.982  1.00 21.07    A   C
ATOM  1775  OD1 ASN A 227     32.223  42.137  51.679  1.00 19.99    A   O
ATOM  1776  ND2 ASN A 227     33.733  40.659  50.916  1.00 19.44    A   N
ATOM  1777  C   ASN A 227     29.428  41.805  50.783  1.00 24.57    A   C
ATOM  1778  O   ASN A 227     29.198  41.005  51.690  1.00 21.91    A   O
ATOM  1779  N   ALA A 228     28.891  43.021  50.741  1.00 23.23    A   N
ATOM  1780  CA  ALA A 228     27.969  43.481  51.776  1.00 26.14    A   C
ATOM  1781  CB  ALA A 228     27.806  45.001  51.699  1.00 22.82    A   C
ATOM  1782  C   ALA A 228     26.611  42.793  51.596  1.00 26.93    A   C
ATOM  1783  O   ALA A 228     26.405  42.077  50.619  1.00 26.75    A   O
ATOM  1784  N   CYS A 229     25.698  43.016  52.541  1.00 29.94    A   N
ATOM  1785  CA  CYS A 229     24.359  42.425  52.508  1.00 34.05    A   C
ATOM  1786  CB  CYS A 229     23.438  43.143  53.508  1.00 36.45    A   C
ATOM  1787  SG  CYS A 229     23.886  42.897  55.243  1.00 48.21    A   S
ATOM  1788  C   CYS A 229     23.730  42.476  51.124  1.00 35.31    A   C
ATOM  1789  O   CYS A 229     23.882  43.451  50.399  1.00 35.27    A   O
ATOM  1790  N   THR A 230     23.030  41.412  50.757  1.00 38.04    A   N
ATOM  1791  CA  THR A 230     22.378  41.380  49.466  1.00 40.97    A   C
ATOM  1792  CB  THR A 230     21.965  39.958  49.076  1.00 42.40    A   C
ATOM  1793  OG1 THR A 230     21.273  39.335  50.163  1.00 45.09    A   O
ATOM  1794  CG2 THR A 230     23.190  39.148  48.730  1.00 43.15    A   C
ATOM  1795  C   THR A 230     21.150  42.269  49.476  1.00 41.97    A   C
ATOM  1796  O   THR A 230     20.887  42.971  48.493  1.00 42.37    A   O
ATOM  1797  N   PHE A 231     20.376  42.232  50.552  1.00 42.74    A   N
ATOM  1798  CA  PHE A 231     19.230  43.108  50.576  1.00 43.96    A   C
ATOM  1799  CB  PHE A 231     17.938  42.321  50.366  1.00 49.35    A   C
ATOM  1800  CG  PHE A 231     17.721  41.990  48.907  1.00 55.66    A   C
ATOM  1801  CD1 PHE A 231     18.494  41.004  48.306  1.00 58.70    A   C
ATOM  1802  CD2 PHE A 231     16.903  42.785  48.088  1.00 58.59    A   C
ATOM  1803  CE1 PHE A 231     18.483  40.801  46.922  1.00 60.69    A   C
ATOM  1804  CE2 PHE A 231     16.879  42.597  46.701  1.00 60.58    A   C
ATOM  1805  CZ  PHE A 231     17.668  41.604  46.113  1.00 60.92    A   C
ATOM  1806  C   PHE A 231     19.335  43.912  51.838  1.00 40.83    A   C
ATOM  1807  O   PHE A 231     18.811  43.567  52.886  1.00 42.69    A   O
ATOM  1808  N   PRO A 232     20.153  44.975  51.722  1.00 35.76    A   N
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Figure 6GG

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ATOM  1809  CD  PRO A 232      20.672  45.196  50.347  1.00 35.27      A   C
ATOM  1810  CA  PRO A 232      20.579  46.028  52.651  1.00 32.93      A   C
ATOM  1811  CB  PRO A 232      21.689  46.764  51.874  1.00 32.41      A   C
ATOM  1812  CG  PRO A 232      21.363  46.497  50.424  1.00 32.47      A   C
ATOM  1813  C   PRO A 232      19.457  46.929  53.137  1.00 29.06      A   C
ATOM  1814  O   PRO A 232      18.456  47.146  52.452  1.00 27.86      A   O
ATOM  1815  N   LYS A 233      19.630  47.440  54.346  1.00 27.89      A   N
ATOM  1816  CA  LYS A 233      18.645  48.314  54.943  1.00 25.66      A   C
ATOM  1817  CB  LYS A 233      18.682  48.188  56.464  1.00 29.61      A   C
ATOM  1818  CG  LYS A 233      18.178  46.843  56.973  1.00 34.08      A   C
ATOM  1819  CD  LYS A 233      18.086  46.829  58.491  1.00 40.01      A   C
ATOM  1820  CE  LYS A 233      19.454  46.996  59.139  1.00 41.92      A   C
ATOM  1821  NZ  LYS A 233      19.351  47.038  60.626  1.00 44.78      A   N
ATOM  1822  C   LYS A 233      18.945  49.739  54.524  1.00 23.25      A   C
ATOM  1823  O   LYS A 233      20.042  50.248  54.738  1.00 20.72      A   O
ATOM  1824  N   VAL A 234      17.959  50.374  53.909  1.00 21.94      A   N
ATOM  1825  CA  VAL A 234      18.122  51.742  53.457  1.00 18.96      A   C
ATOM  1826  CB  VAL A 234      18.171  51.809  51.927  1.00 18.07      A   C
ATOM  1827  CG1 VAL A 234      18.407  53.242  51.484  1.00 15.91      A   C
ATOM  1828  CG2 VAL A 234      19.265  50.884  51.403  1.00 19.03      A   C
ATOM  1829  C   VAL A 234      16.982  52.622  53.945  1.00 19.45      A   C
ATOM  1830  O   VAL A 234      15.810  52.291  53.775  1.00 18.84      A   O
ATOM  1831  N   GLU A 235      17.332  53.749  54.550  1.00 18.70      A   N
ATOM  1832  CA  GLU A 235      16.333  54.682  55.044  1.00 19.65      A   C
ATOM  1833  CB  GLU A 235      16.584  55.029  56.513  1.00 20.87      A   C
ATOM  1834  CG  GLU A 235      16.619  53.849  57.461  1.00 24.25      A   C
ATOM  1835  CD  GLU A 235      16.762  54.287  58.908  1.00 26.71      A   C
ATOM  1836  OE1 GLU A 235      16.924  53.412  59.782  1.00 30.95      A   O
ATOM  1837  OE2 GLU A 235      16.710  55.509  59.174  1.00 28.58      A   O
ATOM  1838  C   GLU A 235      16.433  55.957  54.226  1.00 19.63      A   C
ATOM  1839  O   GLU A 235      17.522  56.339  53.793  1.00 19.08      A   O
ATOM  1840  N   PHE A 236      15.295  56.608  54.008  1.00 16.22      A   N
ATOM  1841  CA  PHE A 236      15.281  57.850  53.260  1.00 15.50      A   C
ATOM  1842  CB  PHE A 236      14.454  57.703  51.985  1.00 16.22      A   C
ATOM  1843  CG  PHE A 236      15.028  56.712  51.008  1.00 16.49      A   C
ATOM  1844  CD1 PHE A 236      14.734  55.352  51.117  1.00 14.80      A   C
ATOM  1845  CD2 PHE A 236      15.906  57.131  50.011  1.00 16.20      A   C
ATOM  1846  CE1 PHE A 236      15.311  54.423  50.249  1.00 16.35      A   C
ATOM  1847  CE2 PHE A 236      16.488  56.213  49.140  1.00 16.85      A   C
ATOM  1848  CZ  PHE A 236      16.191  54.857  49.258  1.00 18.08      A   C
ATOM  1849  C   PHE A 236      14.725  58.953  54.150  1.00 17.81      A   C
ATOM  1850  O   PHE A 236      13.669  58.808  54.771  1.00 17.48      A   O
ATOM  1851  N   HIS A 237      15.473  60.043  54.238  1.00 14.01      A   N
ATOM  1852  CA  HIS A 237      15.077  61.178  55.050  1.00 13.85      A   C
ATOM  1853  CB  HIS A 237      15.976  61.261  56.282  1.00 16.76      A   C
ATOM  1854  CG  HIS A 237      15.871  60.068  57.183  1.00 20.30      A   C
ATOM  1855  CD2 HIS A 237      16.529  58.884  57.176  1.00 22.69      A   C
ATOM  1856  ND1 HIS A 237      14.963  59.994  58.216  1.00 21.64      A   N
ATOM  1857  CE1 HIS A 237      15.065  58.816  58.808  1.00 24.58      A   C
ATOM  1858  NE2 HIS A 237      16.008  58.123  58.196  1.00 24.02      A   N
ATOM  1859  C   HIS A 237      15.240  62.421  54.190  1.00 12.98      A   C
ATOM  1860  O   HIS A 237      15.960  62.402  53.199  1.00 14.24      A   O
ATOM  1861  N   ALA A 238      14.573  63.500  54.571  1.00 14.25      A   N
ATOM  1862  CA  ALA A 238      14.656  64.745  53.822  1.00 14.74      A   C
ATOM  1863  CB  ALA A 238      13.867  64.622  52.523  1.00 13.87      A   C
ATOM  1864  C   ALA A 238      14.105  65.889  54.662  1.00 16.80      A   C
ATOM  1865  O   ALA A 238      13.416  65.662  55.659  1.00 13.41      A   O
ATOM  1866  N   SER A 239      14.419  67.118  54.265  1.00 16.83      A   N
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Figure 6HH

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ATOM  1867  CA  SER A 239     13.934  68.289  54.982  1.00 15.86    A   C
ATOM  1868  CB  SER A 239     14.874  69.472  54.749  1.00 17.78    A   C
ATOM  1869  OG  SER A 239     15.235  69.570  53.382  1.00 15.31    A   O
ATOM  1870  C   SER A 239     12.526  68.628  54.501  1.00 18.27    A   C
ATOM  1871  O   SER A 239     11.851  69.475  55.081  1.00 19.09    A   O
ATOM  1872  N   GLY A 240     12.093  67.950  53.440  1.00 19.12    A   N
ATOM  1873  CA  GLY A 240     10.764  68.172  52.891  1.00 18.85    A   C
ATOM  1874  C   GLY A 240     10.400  67.108  51.872  1.00 20.08    A   C
ATOM  1875  O   GLY A 240     11.262  66.321  51.462  1.00 19.84    A   O
ATOM  1876  N   ASP A 241      9.134  67.065  51.464  1.00 17.58    A   N
ATOM  1877  CA  ASP A 241      8.692  66.077  50.481  1.00 19.46    A   C
ATOM  1878  CB  ASP A 241      9.150  66.501  49.083  1.00 21.27    A   C
ATOM  1879  CG  ASP A 241      8.429  67.738  48.587  1.00 23.85    A   C
ATOM  1880  OD1 ASP A 241      7.247  67.610  48.206  1.00 26.32    A   O
ATOM  1881  OD2 ASP A 241      9.038  68.833  48.591  1.00 21.42    A   O
ATOM  1882  C   ASP A 241      9.257  64.694  50.803  1.00 16.99    A   C
ATOM  1883  O   ASP A 241      9.731  63.987  49.913  1.00 17.49    A   O
ATOM  1884  N   VAL A 242      9.208  64.316  52.076  1.00 15.93    A   N
ATOM  1885  CA  VAL A 242      9.737  63.025  52.516  1.00 14.13    A   C
ATOM  1886  CB  VAL A 242      9.894  62.990  54.052  1.00 17.19    A   C
ATOM  1887  CG1 VAL A 242     10.671  61.740  54.469  1.00 16.23    A   C
ATOM  1888  CG2 VAL A 242     10.612  64.248  54.523  1.00 18.97    A   C
ATOM  1889  C   VAL A 242      8.849  61.864  52.082  1.00 15.60    A   C
ATOM  1890  O   VAL A 242      9.341  60.808  51.660  1.00 12.78    A   O
ATOM  1891  N   ILE A 243      7.540  62.057  52.209  1.00 14.41    A   N
ATOM  1892  CA  ILE A 243      6.577  61.045  51.803  1.00 16.25    A   C
ATOM  1893  CB  ILE A 243      5.125  61.549  52.007  1.00 18.10    A   C
ATOM  1894  CG2 ILE A 243      4.123  60.554  51.414  1.00 20.99    A   C
ATOM  1895  CG1 ILE A 243      4.858  61.747  53.502  1.00 21.18    A   C
ATOM  1896  CD1 ILE A 243      3.485  62.293  53.817  1.00 20.78    A   C
ATOM  1897  C   ILE A 243      6.833  60.787  50.324  1.00 15.05    A   C
ATOM  1898  O   ILE A 243      6.885  59.639  49.878  1.00 16.76    A   O
ATOM  1899  N   TRP A 244      7.005  61.868  49.569  1.00 13.24    A   N
ATOM  1900  CA  TRP A 244      7.270  61.768  48.142  1.00 15.52    A   C
ATOM  1901  CB  TRP A 244      7.343  63.164  47.523  1.00 13.47    A   C
ATOM  1902  CG  TRP A 244      7.510  63.151  46.036  1.00 18.87    A   C
ATOM  1903  CD2 TRP A 244      8.732  63.342  45.312  1.00 17.48    A   C
ATOM  1904  CE2 TRP A 244      8.426  63.232  43.940  1.00 18.22    A   C
ATOM  1905  CE3 TRP A 244     10.057  63.594  45.693  1.00 17.59    A   C
ATOM  1906  CD1 TRP A 244      6.538  62.938  45.099  1.00 18.15    A   C
ATOM  1907  NE1 TRP A 244      7.083  62.988  43.835  1.00 18.29    A   N
ATOM  1908  CZ2 TRP A 244      9.399  63.366  42.943  1.00 20.22    A   C
ATOM  1909  CZ3 TRP A 244     11.024  63.727  44.702  1.00 18.36    A   C
ATOM  1910  CH2 TRP A 244     10.688  63.611  43.342  1.00 18.43    A   C
ATOM  1911  C   TRP A 244      8.590  61.042  47.891  1.00 14.64    A   C
ATOM  1912  O   TRP A 244      8.670  60.149  47.044  1.00 16.51    A   O
ATOM  1913  N   LEU A 245      9.628  61.436  48.623  1.00 13.56    A   N
ATOM  1914  CA  LEU A 245     10.941  60.814  48.459  1.00 12.19    A   C
ATOM  1915  CB  LEU A 245     11.946  61.416  49.444  1.00 11.28    A   C
ATOM  1916  CG  LEU A 245     13.379  60.875  49.342  1.00 11.24    A   C
ATOM  1917  CD1 LEU A 245     13.988  61.289  48.009  1.00 11.74    A   C
ATOM  1918  CD2 LEU A 245     14.223  61.407  50.490  1.00 10.22    A   C
ATOM  1919  C   LEU A 245     10.862  59.301  48.661  1.00 14.05    A   C
ATOM  1920  O   LEU A 245     11.439  58.537  47.884  1.00 12.33    A   O
ATOM  1921  N   GLU A 246     10.144  58.870  49.698  1.00 14.68    A   N
ATOM  1922  CA  GLU A 246     10.000  57.441  49.980  1.00 16.30    A   C
ATOM  1923  CB  GLU A 246      9.198  57.213  51.267  1.00 16.70    A   C
ATOM  1924  CG  GLU A 246      9.938  57.637  52.521  1.00 23.08    A   C
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Figure 6II

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ATOM  1925 CD  GLU A 246     9.544  56.818  53.737  1.00 25.63    A   C
ATOM  1926 OE1 GLU A 246     8.335  56.577  53.927  1.00 24.93    A   O
ATOM  1927 OE2 GLU A 246    10.444  56.423  54.508  1.00 27.10    A   O
ATOM  1928 C   GLU A 246     9.324  56.714  48.828  1.00 15.72    A   C
ATOM  1929 O   GLU A 246     9.691  55.589  48.494  1.00 15.40    A   O
ATOM  1930 N   ARG A 247     8.326  57.359  48.235  1.00 16.57    A   N
ATOM  1931 CA  ARG A 247     7.611  56.790  47.105  1.00 18.74    A   C
ATOM  1932 CB  ARG A 247     6.445  57.710  46.711  1.00 23.10    A   C
ATOM  1933 CG  ARG A 247     5.875  57.451  45.325  1.00 32.32    A   C
ATOM  1934 CD  ARG A 247     4.561  58.204  45.114  1.00 40.32    A   C
ATOM  1935 NE  ARG A 247     4.084  58.117  43.733  1.00 47.44    A   N
ATOM  1936 CZ  ARG A 247     4.569  58.835  42.722  1.00 49.78    A   C
ATOM  1937 NH1 ARG A 247     5.548  59.705  42.931  1.00 51.70    A   N
ATOM  1938 NH2 ARG A 247     4.079  58.682  41.497  1.00 52.43    A   N
ATOM  1939 C   ARG A 247     8.594  56.630  45.941  1.00 17.54    A   C
ATOM  1940 O   ARG A 247     8.654  55.578  45.299  1.00 14.31    A   O
ATOM  1941 N   GLN A 248     9.375  57.672  45.677  1.00 15.93    A   N
ATOM  1942 CA  GLN A 248    10.350  57.608  44.598  1.00 16.24    A   C
ATOM  1943 CB  GLN A 248    11.120  58.929  44.485  1.00 17.33    A   C
ATOM  1944 CG  GLN A 248    10.267  60.119  44.047  1.00 16.22    A   C
ATOM  1945 CD  GLN A 248     9.552  59.879  42.725  1.00 22.44    A   C
ATOM  1946 OE1 GLN A 248    10.184  59.627  41.694  1.00 22.85    A   O
ATOM  1947 NE2 GLN A 248     8.225  59.958  42.749  1.00 24.90    A   N
ATOM  1948 C   GLN A 248    11.324  56.453  44.815  1.00 15.90    A   C
ATOM  1949 O   GLN A 248    11.705  55.768  43.866  1.00 16.87    A   O
ATOM  1950 N   ALA A 249    11.720  56.231  46.065  1.00 15.92    A   N
ATOM  1951 CA  ALA A 249    12.644  55.146  46.384  1.00 15.55    A   C
ATOM  1952 CB  ALA A 249    13.015  55.191  47.857  1.00 16.80    A   C
ATOM  1953 C   ALA A 249    12.032  53.789  46.041  1.00 16.47    A   C
ATOM  1954 O   ALA A 249    12.685  52.943  45.426  1.00 16.21    A   O
ATOM  1955 N   LYS A 250    10.779  53.582  46.438  1.00 16.38    A   N
ATOM  1956 CA  LYS A 250    10.102  52.316  46.159  1.00 18.81    A   C
ATOM  1957 CB  LYS A 250     8.750  52.258  46.880  1.00 20.86    A   C
ATOM  1958 CG  LYS A 250     8.843  52.132  48.394  1.00 26.84    A   C
ATOM  1959 CD  LYS A 250     7.488  51.745  48.988  1.00 31.08    A   C
ATOM  1960 CE  LYS A 250     7.554  51.607  50.507  1.00 31.43    A   C
ATOM  1961 NZ  LYS A 250     7.896  52.899  51.156  1.00 29.87    A   N
ATOM  1962 C   LYS A 250     9.884  52.121  44.661  1.00 18.41    A   C
ATOM  1963 O   LYS A 250    10.073  51.024  44.125  1.00 15.17    A   O
ATOM  1964 N   GLU A 251     9.493  53.200  43.992  1.00 15.62    A   N
ATOM  1965 CA  GLU A 251     9.224  53.167  42.562  1.00 18.32    A   C
ATOM  1966 CB  GLU A 251     8.586  54.486  42.119  1.00 20.33    A   C
ATOM  1967 CG  GLU A 251     7.205  54.758  42.692  1.00 23.48    A   C
ATOM  1968 CD  GLU A 251     6.106  54.036  41.936  1.00 25.23    A   C
ATOM  1969 OE1 GLU A 251     6.415  53.361  40.932  1.00 28.49    A   O
ATOM  1970 OE2 GLU A 251     4.932  54.152  42.341  1.00 25.47    A   O
ATOM  1971 C   GLU A 251    10.448  52.921  41.694  1.00 20.06    A   C
ATOM  1972 O   GLU A 251    10.398  52.121  40.763  1.00 17.23    A   O
ATOM  1973 N   TRP A 252    11.547  53.606  41.997  1.00 19.52    A   N
ATOM  1974 CA  TRP A 252    12.748  53.489  41.175  1.00 20.14    A   C
ATOM  1975 CB  TRP A 252    13.276  54.885  40.832  1.00 18.05    A   C
ATOM  1976 CG  TRP A 252    12.305  55.710  40.043  1.00 18.22    A   C
ATOM  1977 CD2 TRP A 252    12.039  55.607  38.640  1.00 20.57    A   C
ATOM  1978 CE2 TRP A 252    11.017  56.533  38.339  1.00 20.85    A   C
ATOM  1979 CE3 TRP A 252    12.564  54.818  37.607  1.00 21.87    A   C
ATOM  1980 CD1 TRP A 252    11.460  56.669  40.523  1.00 17.88    A   C
ATOM  1981 NE1 TRP A 252    10.683  57.168  39.508  1.00 17.77    A   N
ATOM  1982 CZ2 TRP A 252    10.506  56.697  37.041  1.00 22.03    A   C
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Figure 6JJ

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ATOM  1983 CZ3 TRP A 252     12.055  54.978  36.314  1.00 21.57    A   C
ATOM  1984 CH2 TRP A 252     11.036  55.913  36.045  1.00 22.86    A   C
ATOM  1985 C  TRP A 252      13.902  52.641  41.688  1.00 22.39    A   C
ATOM  1986 O  TRP A 252      14.680  52.122  40.886  1.00 23.72    A   O
ATOM  1987 N  LEU A 253      14.024  52.504  43.003  1.00 22.18    A   N
ATOM  1988 CA  LEU A 253     15.106  51.717  43.588  1.00 25.35    A   C
ATOM  1989 CB  LEU A 253     15.809  52.524  44.680  1.00 20.44    A   C
ATOM  1990 CG  LEU A 253     16.355  53.904  44.285  1.00 21.92    A   C
ATOM  1991 CD1 LEU A 253     16.785  54.649  45.532  1.00 18.63    A   C
ATOM  1992 CD2 LEU A 253     17.530  53.758  43.316  1.00 20.79    A   C
ATOM  1993 C  LEU A 253      14.583  50.401  44.168  1.00 29.73    A   C
ATOM  1994 O  LEU A 253      15.357  49.570  44.647  1.00 31.04    A   O
ATOM  1995 N  LYS A 254      13.267  50.219  44.121  1.00 33.91    A   N
ATOM  1996 CA  LYS A 254     12.638  49.007  44.631  1.00 39.79    A   C
ATOM  1997 CB  LYS A 254     13.102  47.795  43.812  1.00 43.18    A   C
ATOM  1998 CG  LYS A 254     12.330  46.518  44.102  1.00 51.27    A   C
ATOM  1999 CD  LYS A 254     12.747  45.377  43.181  1.00 56.67    A   C
ATOM  2000 CE  LYS A 254     11.928  44.121  43.464  1.00 59.29    A   C
ATOM  2001 NZ  LYS A 254     10.463  44.368  43.307  1.00 62.20    A   N
ATOM  2002 C  LYS A 254      12.967  48.805  46.110  1.00 41.24    A   C
ATOM  2003 O  LYS A 254      13.111  47.678  46.586  1.00 42.02    A   O
ATOM  2004 N  LEU A 255      13.091  49.911  46.834  1.00 42.21    A   N
ATOM  2005 CA  LEU A 255     13.396  49.856  48.255  1.00 43.88    A   C
ATOM  2006 CB  LEU A 255     14.643  50.687  48.560  1.00 41.85    A   C
ATOM  2007 CG  LEU A 255     15.934  50.186  47.910  1.00 40.40    A   C
ATOM  2008 CD1 LEU A 255     17.065  51.143  48.229  1.00 40.11    A   C
ATOM  2009 CD2 LEU A 255     16.258  48.788  48.412  1.00 39.40    A   C
ATOM  2010 C  LEU A 255      12.211  50.365  49.070  1.00 46.21    A   C
ATOM  2011 O  LEU A 255      12.350  51.427  49.715  1.00 47.30    A   O
ATOM  2012 OXT LEU A 255     11.152  49.696  49.044  1.00 48.09    A   O
ATOM  2013 CB  MET B  1       3.272 103.508  55.905  1.00 23.27    B   C
ATOM  2014 CG  MET B  1       3.026 102.116  56.484  1.00 25.31    B   C
ATOM  2015 SD  MET B  1       1.613 101.253  55.747  1.00 29.32    B   S
ATOM  2016 CE  MET B  1       0.239 102.076  56.594  1.00 27.48    B   C
ATOM  2017 C  MET B  1        5.739 103.357  56.203  1.00 22.82    B   C
ATOM  2018 O  MET B  1        6.391 103.503  55.166  1.00 21.44    B   O
ATOM  2019 N  MET B  1        4.661 105.565  55.875  1.00 22.28    B   N
ATOM  2020 CA  MET B  1       4.509 104.211  56.478  1.00 22.89    B   C
ATOM  2021 N  LYS B  2        6.057 102.479  57.148  1.00 22.63    B   N
ATOM  2022 CA  LYS B  2       7.185 101.568  57.010  1.00 21.27    B   C
ATOM  2023 CB  LYS B  2       8.060 101.591  58.260  1.00 21.29    B   C
ATOM  2024 CG  LYS B  2       9.273 100.675  58.156  1.00 18.62    B   C
ATOM  2025 CD  LYS B  2      10.097 100.705  59.419  1.00 18.80    B   C
ATOM  2026 CE  LYS B  2      11.414  99.983  59.213  1.00 19.94    B   C
ATOM  2027 NZ  LYS B  2      12.203  99.908  60.474  1.00 21.20    B   N
ATOM  2028 C  LYS B  2        6.610 100.169  56.822  1.00 19.67    B   C
ATOM  2029 O  LYS B  2        5.903  99.661  57.692  1.00 20.03    B   O
ATOM  2030 N  ILE B  3        6.915  99.545  55.689  1.00 18.60    B   N
ATOM  2031 CA  ILE B  3       6.395  98.213  55.410  1.00 16.13    B   C
ATOM  2032 CB  ILE B  3       5.409  98.250  54.232  1.00 18.20    B   C
ATOM  2033 CG2 ILE B  3       4.281  99.237  54.516  1.00 15.72    B   C
ATOM  2034 CG1 ILE B  3       6.156  98.669  52.964  1.00 17.99    B   C
ATOM  2035 CD1 ILE B  3       5.909  97.772  51.772  1.00 20.13    B   C
ATOM  2036 C  ILE B  3        7.476  97.190  55.062  1.00 17.01    B   C
ATOM  2037 O  ILE B  3        8.637  97.535  54.820  1.00 13.35    B   O
ATOM  2038 N  GLY B  4        7.072  95.924  55.046  1.00 15.79    B   N
ATOM  2039 CA  GLY B  4       7.982  94.859  54.678  1.00 13.12    B   C
ATOM  2040 C  GLY B  4        7.474  94.217  53.401  1.00 12.84    B   C
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Figure 6KK

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ATOM  2041  O   GLY B  4      6.271  94.248  53.123  1.00 12.27      B   O
ATOM  2042  N   VAL B  5      8.387  93.670  52.602  1.00 11.41      B   N
ATOM  2043  CA  VAL B  5      8.024  92.982  51.362  1.00 12.46      B   C
ATOM  2044  CB  VAL B  5      8.471  93.755  50.092  1.00 11.43      B   C
ATOM  2045  CG1 VAL B  5      8.281  92.886  48.860  1.00 10.57      B   C
ATOM  2046  CG2 VAL B  5      7.646  95.026  49.938  1.00 13.41      B   C
ATOM  2047  C   VAL B  5      8.745  91.641  51.404  1.00 11.84      B   C
ATOM  2048  O   VAL B  5      9.964  91.591  51.565  1.00 13.84      B   O
ATOM  2049  N   PHE B  6      7.989  90.559  51.277  1.00 11.52      B   N
ATOM  2050  CA  PHE B  6      8.571  89.222  51.330  1.00 12.00      B   C
ATOM  2051  CB  PHE B  6      7.930  88.429  52.471  1.00 14.01      B   C
ATOM  2052  CG  PHE B  6      8.313  86.975  52.485  1.00 15.68      B   C
ATOM  2053  CD1 PHE B  6      9.650  86.598  52.576  1.00 15.79      B   C
ATOM  2054  CD2 PHE B  6      7.340  85.983  52.403  1.00 17.28      B   C
ATOM  2055  CE1 PHE B  6     10.017  85.251  52.584  1.00 15.22      B   C
ATOM  2056  CE2 PHE B  6      7.699  84.628  52.411  1.00 18.59      B   C
ATOM  2057  CZ  PHE B  6      9.044  84.268  52.502  1.00 15.23      B   C
ATOM  2058  C   PHE B  6      8.440  88.410  50.046  1.00 12.99      B   C
ATOM  2059  O   PHE B  6      7.396  88.412  49.400  1.00 13.52      B   O
ATOM  2060  N   ASP B  7      9.512  87.707  49.695  1.00 13.22      B   N
ATOM  2061  CA  ASP B  7      9.533  86.839  48.523  1.00 12.28      B   C
ATOM  2062  CB  ASP B  7      9.914  87.600  47.254  1.00 12.10      B   C
ATOM  2063  CG  ASP B  7      9.838  86.727  46.018  1.00 11.16      B   C
ATOM  2064  OD1 ASP B  7      8.773  86.111  45.800  1.00 11.05      B   O
ATOM  2065  OD2 ASP B  7     10.835  86.652  45.265  1.00 15.46      B   O
ATOM  2066  C   ASP B  7     10.544  85.730  48.749  1.00 12.97      B   C
ATOM  2067  O   ASP B  7     11.402  85.831  49.626  1.00 14.91      B   O
ATOM  2068  N   SER B  8     10.444  84.670  47.953  1.00 13.64      B   N
ATOM  2069  CA  SER B  8     11.367  83.551  48.076  1.00 13.32      B   C
ATOM  2070  CB  SER B  8     10.870  82.357  47.246  1.00 11.76      B   C
ATOM  2071  OG  SER B  8     10.643  82.716  45.892  1.00 12.59      B   O
ATOM  2072  C   SER B  8     12.760  83.979  47.618  1.00 12.86      B   C
ATOM  2073  O   SER B  8     13.760  83.328  47.931  1.00 15.56      B   O
ATOM  2074  N   GLY B  9     12.826  85.088  46.888  1.00 14.15      B   N
ATOM  2075  CA  GLY B  9     14.113  85.565  46.418  1.00 11.94      B   C
ATOM  2076  C   GLY B  9     14.060  86.923  45.751  1.00 13.28      B   C
ATOM  2077  O   GLY B  9     13.420  87.855  46.255  1.00 11.42      B   O
ATOM  2078  N   VAL B 10     14.731  87.031  44.608  1.00 11.70      B   N
ATOM  2079  CA  VAL B 10     14.793  88.283  43.848  1.00 13.19      B   C
ATOM  2080  CB  VAL B 10     16.035  88.301  42.931  1.00 11.94      B   C
ATOM  2081  CG1 VAL B 10     15.956  87.149  41.948  1.00 17.01      B   C
ATOM  2082  CG2 VAL B 10     16.148  89.633  42.200  1.00 12.63      B   C
ATOM  2083  C   VAL B 10     13.546  88.495  42.995  1.00 12.34      B   C
ATOM  2084  O   VAL B 10     13.267  89.604  42.550  1.00 14.01      B   O
ATOM  2085  N   GLY B 11     12.794  87.426  42.768  1.00 12.08      B   N
ATOM  2086  CA  GLY B 11     11.591  87.540  41.957  1.00 14.90      B   C
ATOM  2087  C   GLY B 11     10.634  88.640  42.373  1.00 12.77      B   C
ATOM  2088  O   GLY B 11     10.004  89.278  41.524  1.00 13.23      B   O
ATOM  2089  N   GLY B 12     10.524  88.861  43.679  1.00 13.56      B   N
ATOM  2090  CA  GLY B 12      9.639  89.887  44.198  1.00 15.76      B   C
ATOM  2091  C   GLY B 12      9.917  91.279  43.659  1.00 15.26      B   C
ATOM  2092  O   GLY B 12      9.141  92.213  43.899  1.00 15.12      B   O
ATOM  2093  N   PHE B 13     11.024  91.426  42.937  1.00 12.59      B   N
ATOM  2094  CA  PHE B 13     11.376  92.713  42.360  1.00 14.03      B   C
ATOM  2095  CB  PHE B 13     12.702  92.620  41.589  1.00 14.04      B   C
ATOM  2096  CG  PHE B 13     13.929  92.823  42.446  1.00 14.87      B   C
ATOM  2097  CD1 PHE B 13     15.133  93.231  41.868  1.00 16.32      B   C
ATOM  2098  CD2 PHE B 13     13.883  92.629  43.823  1.00 14.64      B   C
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Figure 6LL

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ATOM  2099 CE1 PHE B 13     16.272  93.448  42.651  1.00 13.70      B   C
ATOM  2100 CE2 PHE B 13     15.013  92.842  44.614  1.00 13.54      B   C
ATOM  2101 CZ  PHE B 13     16.210  93.254  44.025  1.00 15.35      B   C
ATOM  2102 C   PHE B 13     10.260  93.184  41.425  1.00 14.72      B   C
ATOM  2103 O   PHE B 13     10.013  94.380  41.301  1.00 12.42      B   O
ATOM  2104 N   SER B 14      9.580  92.243  40.775  1.00 14.71      B   N
ATOM  2105 CA  SER B 14      8.494  92.600  39.860  1.00 14.65      B   C
ATOM  2106 CB  SER B 14      7.918  91.349  39.187  1.00 14.09      B   C
ATOM  2107 OG  SER B 14      7.405  90.436  40.135  1.00 13.06      B   O
ATOM  2108 C   SER B 14      7.380  93.355  40.587  1.00 14.07      B   C
ATOM  2109 O   SER B 14      6.688  94.187  39.994  1.00 13.89      B   O
ATOM  2110 N   VAL B 15      7.212  93.064  41.872  1.00 14.55      B   N
ATOM  2111 CA  VAL B 15      6.196  93.737  42.675  1.00 14.09      B   C
ATOM  2112 CB  VAL B 15      5.675  92.827  43.814  1.00 12.74      B   C
ATOM  2113 CG1 VAL B 15      4.705  93.600  44.698  1.00 13.09      B   C
ATOM  2114 CG2 VAL B 15      4.971  91.604  43.224  1.00 11.77      B   C
ATOM  2115 C   VAL B 15      6.789  95.003  43.283  1.00 14.70      B   C
ATOM  2116 O   VAL B 15      6.145  96.052  43.307  1.00 13.74      B   O
ATOM  2117 N   LEU B 16      8.022  94.903  43.769  1.00 13.69      B   N
ATOM  2118 CA  LEU B 16      8.679  96.048  44.384  1.00 14.26      B   C
ATOM  2119 CB  LEU B 16     10.082  95.662  44.863  1.00 13.66      B   C
ATOM  2120 CG  LEU B 16     10.940  96.793  45.448  1.00 14.21      B   C
ATOM  2121 CD1 LEU B 16     10.201  97.451  46.605  1.00 12.59      B   C
ATOM  2122 CD2 LEU B 16     12.280  96.242  45.905  1.00 12.19      B   C
ATOM  2123 C   LEU B 16      8.757  97.212  43.401  1.00 16.29      B   C
ATOM  2124 O   LEU B 16      8.614  98.373  43.787  1.00 16.57      B   O
ATOM  2125 N   LYS B 17      8.984  96.896  42.129  1.00 17.51      B   N
ATOM  2126 CA  LYS B 17      9.069  97.927  41.099  1.00 19.45      B   C
ATOM  2127 CB  LYS B 17      9.349  97.298  39.733  1.00 19.95      B   C
ATOM  2128 CG  LYS B 17      9.302  98.291  38.578  1.00 24.40      B   C
ATOM  2129 CD  LYS B 17      9.568  97.608  37.245  1.00 29.79      B   C
ATOM  2130 CE  LYS B 17      9.472  98.586  36.081  1.00 33.15      B   C
ATOM  2131 NZ  LYS B 17      9.808  97.925  34.784  1.00 35.04      B   N
ATOM  2132 C   LYS B 17      7.769  98.722  41.038  1.00 19.40      B   C
ATOM  2133 O   LYS B 17      7.788  99.950  40.985  1.00 18.81      B   O
ATOM  2134 N   SER B 18      6.642  98.018  41.042  1.00 18.29      B   N
ATOM  2135 CA  SER B 18      5.344  98.675  40.997  1.00 18.21      B   C
ATOM  2136 CB  SER B 18      4.221  97.636  40.941  1.00 17.21      B   C
ATOM  2137 OG  SER B 18      4.357  96.808  39.798  1.00 17.80      B   O
ATOM  2138 C   SER B 18      5.162  99.561  42.222  1.00 19.88      B   C
ATOM  2139 O   SER B 18      4.720 100.703  42.112  1.00 17.77      B   O
ATOM  2140 N   LEU B 19      5.510  99.030  43.391  1.00 19.41      B   N
ATOM  2141 CA  LEU B 19      5.379  99.785  44.629  1.00 19.33      B   C
ATOM  2142 CB  LEU B 19      5.839  98.936  45.817  1.00 18.90      B   C
ATOM  2143 CG  LEU B 19      5.085  97.622  46.027  1.00 20.11      B   C
ATOM  2144 CD1 LEU B 19      5.701  96.850  47.188  1.00 18.40      B   C
ATOM  2145 CD2 LEU B 19      3.612  97.919  46.289  1.00 17.29      B   C
ATOM  2146 C   LEU B 19      6.205 101.063  44.564  1.00 18.96      B   C
ATOM  2147 O   LEU B 19      5.722 102.145  44.897  1.00 19.77      B   O
ATOM  2148 N   LEU B 20      7.455 100.930  44.136  1.00 19.62      B   N
ATOM  2149 CA  LEU B 20      8.355 102.071  44.024  1.00 20.54      B   C
ATOM  2150 CB  LEU B 20      9.736 101.605  43.548  1.00 19.03      B   C
ATOM  2151 CG  LEU B 20     10.562 100.763  44.529  1.00 21.61      B   C
ATOM  2152 CD1 LEU B 20     11.789 100.217  43.824  1.00 17.66      B   C
ATOM  2153 CD2 LEU B 20     10.968 101.613  45.731  1.00 17.70      B   C
ATOM  2154 C   LEU B 20      7.821 103.148  43.077  1.00 21.80      B   C
ATOM  2155 O   LEU B 20      7.864 104.334  43.397  1.00 24.32      B   O
ATOM  2156 N   LYS B 21      7.321 102.736  41.916  1.00 22.92      B   N
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Figure 6MM

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ATOM  2157 CA  LYS B 21     6.789 103.680  40.932  1.00 25.60    B   C
ATOM  2158 CB  LYS B 21     6.334 102.934  39.671  1.00 29.64    B   C
ATOM  2159 CG  LYS B 21     7.412 102.050  39.049  1.00 39.78    B   C
ATOM  2160 CD  LYS B 21     6.819 100.964  38.139  1.00 45.78    B   C
ATOM  2161 CE  LYS B 21     6.314 101.521  36.813  1.00 49.52    B   C
ATOM  2162 NZ  LYS B 21     7.428 101.970  35.926  1.00 52.40    B   N
ATOM  2163 C   LYS B 21     5.610 104.455  41.513  1.00 24.12    B   C
ATOM  2164 O   LYS B 21     5.461 105.652  41.270  1.00 21.99    B   O
ATOM  2165 N   ALA B 22     4.775 103.762  42.281  1.00 22.32    B   N
ATOM  2166 CA  ALA B 22     3.602 104.378  42.889  1.00 23.02    B   C
ATOM  2167 CB  ALA B 22     2.619 103.299  43.321  1.00 21.51    B   C
ATOM  2168 C   ALA B 22     3.950 105.279  44.074  1.00 25.48    B   C
ATOM  2169 O   ALA B 22     3.082 105.975  44.602  1.00 26.34    B   O
ATOM  2170 N   ARG B 23     5.214 105.264  44.489  1.00 26.06    B   N
ATOM  2171 CA  ARG B 23     5.674 106.090  45.606  1.00 28.97    B   C
ATOM  2172 CB  ARG B 23     5.794 107.556  45.170  1.00 33.33    B   C
ATOM  2173 CG  ARG B 23     6.504 107.770  43.850  1.00 41.37    B   C
ATOM  2174 CD  ARG B 23     6.349 109.205  43.378  1.00 47.44    B   C
ATOM  2175 NE  ARG B 23     6.782 109.366  41.992  1.00 56.48    B   N
ATOM  2176 CZ  ARG B 23     6.602 110.472  41.275  1.00 59.85    B   C
ATOM  2177 NH1 ARG B 23     5.998 111.520  41.819  1.00 63.01    B   N
ATOM  2178 NH2 ARG B 23     7.019 110.529  40.015  1.00 61.13    B   N
ATOM  2179 C   ARG B 23     4.697 106.012  46.774  1.00 27.89    B   C
ATOM  2180 O   ARG B 23     4.246 107.042  47.276  1.00 27.91    B   O
ATOM  2181 N   LEU B 24     4.373 104.797  47.205  1.00 25.94    B   N
ATOM  2182 CA  LEU B 24     3.430 104.611  48.303  1.00 24.48    B   C
ATOM  2183 CB  LEU B 24     2.653 103.301  48.118  1.00 22.57    B   C
ATOM  2184 CG  LEU B 24     1.822 103.103  46.847  1.00 24.84    B   C
ATOM  2185 CD1 LEU B 24     1.067 101.779  46.942  1.00 23.08    B   C
ATOM  2186 CD2 LEU B 24     0.842 104.266  46.671  1.00 23.49    B   C
ATOM  2187 C   LEU B 24     4.048 104.617  49.699  1.00 24.22    B   C
ATOM  2188 O   LEU B 24     3.445 105.126  50.641  1.00 25.35    B   O
ATOM  2189 N   PHE B 25     5.250 104.068  49.842  1.00 25.14    B   N
ATOM  2190 CA  PHE B 25     5.865 103.997  51.161  1.00 25.20    B   C
ATOM  2191 CB  PHE B 25     6.078 102.531  51.530  1.00 24.64    B   C
ATOM  2192 CG  PHE B 25     4.886 101.665  51.251  1.00 23.70    B   C
ATOM  2193 CD1 PHE B 25     4.849 100.851  50.123  1.00 23.04    B   C
ATOM  2194 CD2 PHE B 25     3.788 101.685  52.098  1.00 22.47    B   C
ATOM  2195 CE1 PHE B 25     3.729 100.070  49.845  1.00 20.01    B   C
ATOM  2196 CE2 PHE B 25     2.666 100.910  51.828  1.00 22.66    B   C
ATOM  2197 CZ  PHE B 25     2.637 100.100  50.697  1.00 21.24    B   C
ATOM  2198 C   PHE B 25     7.164 104.758  51.361  1.00 25.96    B   C
ATOM  2199 O   PHE B 25     8.020 104.796  50.482  1.00 28.54    B   O
ATOM  2200 N   ASP B 26     7.308 105.355  52.540  1.00 26.35    B   N
ATOM  2201 CA  ASP B 26     8.512 106.108  52.872  1.00 28.67    B   C
ATOM  2202 CB  ASP B 26     8.300 106.958  54.130  1.00 31.57    B   C
ATOM  2203 CG  ASP B 26     7.335 108.101  53.907  1.00 33.21    B   C
ATOM  2204 OD1 ASP B 26     7.429 108.753  52.844  1.00 33.40    B   O
ATOM  2205 OD2 ASP B 26     6.495 108.352  54.800  1.00 37.72    B   O
ATOM  2206 C   ASP B 26     9.697 105.186  53.109  1.00 25.51    B   C
ATOM  2207 O   ASP B 26    10.840 105.567  52.877  1.00 22.85    B   O
ATOM  2208 N   GLU B 27     9.421 103.974  53.581  1.00 24.08    B   N
ATOM  2209 CA  GLU B 27    10.483 103.013  53.859  1.00 21.60    B   C
ATOM  2210 CB  GLU B 27    10.964 103.179  55.305  1.00 22.98    B   C
ATOM  2211 CG  GLU B 27    11.869 102.071  55.800  1.00 25.73    B   C
ATOM  2212 CD  GLU B 27    12.636 102.459  57.051  1.00 30.40    B   C
ATOM  2213 OE1 GLU B 27    12.088 103.219  57.883  1.00 28.18    B   O
ATOM  2214 OE2 GLU B 27    13.785 101.993  57.207  1.00 28.75    B   O
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Figure 6NN

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ATOM  2215 C   GLU B 27    10.036 101.576  53.601  1.00 19.70    B   C
ATOM  2216 O   GLU B 27     8.919 101.184  53.948  1.00 17.68    B   O
ATOM  2217 N   ILE B 28    10.926 100.795  52.995  1.00 16.91    B   N
ATOM  2218 CA  ILE B 28    10.630  99.407  52.651  1.00 14.07    B   C
ATOM  2219 CB  ILE B 28    10.394  99.276  51.121  1.00 15.11    B   C
ATOM  2220 CG2 ILE B 28    10.279  97.816  50.711  1.00 15.06    B   C
ATOM  2221 CG1 ILE B 28     9.124 100.034  50.732  1.00 15.08    B   C
ATOM  2222 CD1 ILE B 28     8.920 100.162  49.218  1.00 17.55    B   C
ATOM  2223 C   ILE B 28    11.740  98.446  53.069  1.00 14.73    B   C
ATOM  2224 O   ILE B 28    12.925  98.694  52.825  1.00 14.43    B   O
ATOM  2225 N   ILE B 29    11.348  97.357  53.720  1.00 13.73    B   N
ATOM  2226 CA  ILE B 29    12.299  96.338  54.143  1.00 15.11    B   C
ATOM  2227 CB  ILE B 29    12.113  95.957  55.636  1.00 14.64    B   C
ATOM  2228 CG2 ILE B 29    13.231  95.012  56.077  1.00 13.07    B   C
ATOM  2229 CG1 ILE B 29    12.129  97.214  56.521  1.00 16.50    B   C
ATOM  2230 CD1 ILE B 29    13.462  97.949  56.554  1.00 12.57    B   C
ATOM  2231 C   ILE B 29    11.989  95.121  53.262  1.00 14.26    B   C
ATOM  2232 O   ILE B 29    10.960  94.460  53.438  1.00 16.06    B   O
ATOM  2233 N   TYR B 30    12.857  94.855  52.293  1.00 12.97    B   N
ATOM  2234 CA  TYR B 30    12.667  93.728  51.382  1.00 12.66    B   C
ATOM  2235 CB  TYR B 30    13.095  94.117  49.957  1.00 11.95    B   C
ATOM  2236 CG  TYR B 30    12.831  93.042  48.913  1.00 11.71    B   C
ATOM  2237 CD1 TYR B 30    11.703  93.097  48.096  1.00  9.69    B   C
ATOM  2238 CE1 TYR B 30    11.441  92.100  47.149  1.00 12.54    B   C
ATOM  2239 CD2 TYR B 30    13.700  91.958  48.762  1.00 12.15    B   C
ATOM  2240 CE2 TYR B 30    13.449  90.953  47.817  1.00 14.27    B   C
ATOM  2241 CZ  TYR B 30    12.319  91.033  47.014  1.00 14.57    B   C
ATOM  2242 OH  TYR B 30    12.078  90.061  46.070  1.00 11.66    B   O
ATOM  2243 C   TYR B 30    13.473  92.516  51.842  1.00 15.13    B   C
ATOM  2244 O   TYR B 30    14.673  92.624  52.115  1.00 17.82    B   O
ATOM  2245 N   TYR B 31    12.812  91.364  51.932  1.00 13.53    B   N
ATOM  2246 CA  TYR B 31    13.488  90.144  52.350  1.00 13.30    B   C
ATOM  2247 CB  TYR B 31    13.063  89.742  53.773  1.00 14.35    B   C
ATOM  2248 CG  TYR B 31    13.588  88.381  54.209  1.00 13.93    B   C
ATOM  2249 CD1 TYR B 31    14.955  88.143  54.318  1.00 13.81    B   C
ATOM  2250 CE1 TYR B 31    15.446  86.887  54.682  1.00 16.52    B   C
ATOM  2251 CD2 TYR B 31    12.712  87.326  54.481  1.00 15.49    B   C
ATOM  2252 CE2 TYR B 31    13.191  86.064  54.850  1.00 17.62    B   C
ATOM  2253 CZ  TYR B 31    14.563  85.852  54.946  1.00 14.49    B   C
ATOM  2254 OH  TYR B 31    15.047  84.611  55.304  1.00 14.75    B   O
ATOM  2255 C   TYR B 31    13.188  89.005  51.382  1.00 11.69    B   C
ATOM  2256 O   TYR B 31    12.032  88.657  51.153  1.00 12.79    B   O
ATOM  2257 N   GLY B 32    14.246  88.440  50.812  1.00 12.78    B   N
ATOM  2258 CA  GLY B 32    14.093  87.327  49.896  1.00 11.28    B   C
ATOM  2259 C   GLY B 32    14.761  86.117  50.522  1.00 13.78    B   C
ATOM  2260 O   GLY B 32    15.950  86.162  50.839  1.00 11.17    B   O
ATOM  2261 N   ASP B 33    14.002  85.040  50.710  1.00 14.25    B   N
ATOM  2262 CA  ASP B 33    14.540  83.819  51.306  1.00 15.29    B   C
ATOM  2263 CB  ASP B 33    13.391  82.987  51.885  1.00 13.57    B   C
ATOM  2264 CG  ASP B 33    13.871  81.730  52.589  1.00 14.42    B   C
ATOM  2265 OD1 ASP B 33    15.034  81.702  53.046  1.00 14.38    B   O
ATOM  2266 OD2 ASP B 33    13.077  80.773  52.695  1.00 14.44    B   O
ATOM  2267 C   ASP B 33    15.288  83.049  50.226  1.00 14.09    B   C
ATOM  2268 O   ASP B 33    15.027  81.867  49.980  1.00 12.43    B   O
ATOM  2269 N   SER B 34    16.238  83.739  49.597  1.00 14.94    B   N
ATOM  2270 CA  SER B 34    17.016  83.186  48.490  1.00 14.92    B   C
ATOM  2271 CB  SER B 34    17.941  84.268  47.908  1.00 13.20    B   C
ATOM  2272 OG  SER B 34    18.886  84.714  48.863  1.00 14.39    B   O
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Figure 6OO

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ATOM  2273  C   SER B  34     17.821  81.924  48.772  1.00 14.53      B   C
ATOM  2274  O   SER B  34     18.348  81.308  47.849  1.00 12.91      B   O
ATOM  2275  N   ALA B  35     17.930  81.535  50.034  1.00 13.97      B   N
ATOM  2276  CA  ALA B  35     18.664  80.317  50.345  1.00 15.25      B   C
ATOM  2277  CB  ALA B  35     19.050  80.297  51.820  1.00 15.69      B   C
ATOM  2278  C   ALA B  35     17.801  79.101  50.023  1.00 15.43      B   C
ATOM  2279  O   ALA B  35     18.321  78.010  49.776  1.00 13.55      B   O
ATOM  2280  N   ARG B  36     16.484  79.296  50.000  1.00 13.78      B   N
ATOM  2281  CA  ARG B  36     15.567  78.185  49.777  1.00 14.22      B   C
ATOM  2282  CB  ARG B  36     14.697  78.023  51.027  1.00 13.17      B   C
ATOM  2283  CG  ARG B  36     15.541  77.986  52.303  1.00 13.84      B   C
ATOM  2284  CD  ARG B  36     14.775  77.513  53.520  1.00 16.20      B   C
ATOM  2285  NE  ARG B  36     13.830  78.511  54.012  1.00 13.15      B   N
ATOM  2286  CZ  ARG B  36     13.310  78.500  55.235  1.00 14.54      B   C
ATOM  2287  NH1 ARG B  36     13.642  77.542  56.090  1.00 13.26      B   N
ATOM  2288  NH2 ARG B  36     12.468  79.454  55.613  1.00 15.47      B   N
ATOM  2289  C   ARG B  36     14.703  78.235  48.517  1.00 14.96      B   C
ATOM  2290  O   ARG B  36     13.971  77.288  48.220  1.00 16.93      B   O
ATOM  2291  N   VAL B  37     14.791  79.328  47.770  1.00 14.56      B   N
ATOM  2292  CA  VAL B  37     14.036  79.461  46.530  1.00 15.83      B   C
ATOM  2293  CB  VAL B  37     14.327  80.840  45.875  1.00 16.33      B   C
ATOM  2294  CG1 VAL B  37     15.775  80.909  45.422  1.00 16.98      B   C
ATOM  2295  CG2 VAL B  37     13.379  81.093  44.719  1.00 16.47      B   C
ATOM  2296  C   VAL B  37     14.452  78.312  45.587  1.00 14.68      B   C
ATOM  2297  O   VAL B  37     15.615  77.895  45.575  1.00 15.45      B   O
ATOM  2298  N   PRO B  38     13.511  77.780  44.790  1.00 14.64      B   N
ATOM  2299  CD  PRO B  38     13.845  76.783  43.755  1.00 11.60      B   C
ATOM  2300  CA  PRO B  38     12.102  78.160  44.696  1.00 14.93      B   C
ATOM  2301  CB  PRO B  38     11.743  77.754  43.271  1.00 13.51      B   C
ATOM  2302  CG  PRO B  38     12.485  76.470  43.123  1.00 15.17      B   C
ATOM  2303  C   PRO B  38     11.191  77.489  45.710  1.00 15.27      B   C
ATOM  2304  O   PRO B  38     11.510  76.437  46.274  1.00 13.54      B   O
ATOM  2305  N   TYR B  39     10.043  78.118  45.915  1.00 13.69      B   N
ATOM  2306  CA  TYR B  39      9.013  77.623  46.811  1.00 13.90      B   C
ATOM  2307  CB  TYR B  39      8.268  78.798  47.444  1.00 13.72      B   C
ATOM  2308  CG  TYR B  39      8.922  79.471  48.624  1.00 10.70      B   C
ATOM  2309  CD1 TYR B  39     10.268  79.261  48.937  1.00 10.84      B   C
ATOM  2310  CE1 TYR B  39     10.860  79.906  50.023  1.00 12.25      B   C
ATOM  2311  CD2 TYR B  39      8.186  80.344  49.426  1.00 12.79      B   C
ATOM  2312  CE2 TYR B  39      8.766  80.996  50.514  1.00 12.39      B   C
ATOM  2313  CZ  TYR B  39     10.104  80.772  50.809  1.00 13.35      B   C
ATOM  2314  OH  TYR B  39     10.674  81.405  51.893  1.00 12.01      B   O
ATOM  2315  C   TYR B  39      7.997  76.821  45.987  1.00 14.02      B   C
ATOM  2316  O   TYR B  39      7.451  75.827  46.455  1.00 15.23      B   O
ATOM  2317  N   GLY B  40      7.752  77.290  44.765  1.00 16.75      B   N
ATOM  2318  CA  GLY B  40      6.768  76.686  43.874  1.00 16.84      B   C
ATOM  2319  C   GLY B  40      6.860  75.212  43.525  1.00 16.65      B   C
ATOM  2320  O   GLY B  40      5.886  74.620  43.049  1.00 14.08      B   O
ATOM  2321  N   THR B  41      8.017  74.611  43.766  1.00 15.91      B   N
ATOM  2322  CA  THR B  41      8.225  73.204  43.440  1.00 16.59      B   C
ATOM  2323  CB  THR B  41      9.636  72.990  42.900  1.00 16.07      B   C
ATOM  2324  OG1 THR B  41     10.580  73.477  43.861  1.00 15.88      B   O
ATOM  2325  CG2 THR B  41      9.817  73.737  41.592  1.00 19.86      B   C
ATOM  2326  C   THR B  41      8.072  72.320  44.659  1.00 16.87      B   C
ATOM  2327  O   THR B  41      8.245  71.099  44.584  1.00 18.68      B   O
ATOM  2328  N   LYS B  42      7.742  72.939  45.783  1.00 16.57      B   N
ATOM  2329  CA  LYS B  42      7.647  72.178  47.002  1.00 16.66      B   C
ATOM  2330  CB  LYS B  42      8.592  72.768  48.035  1.00 15.39      B   C
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Figure 6PP

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ATOM  2331 CG  LYS B 42     10.049  72.613  47.578  1.00 16.40    B   C
ATOM  2332 CD  LYS B 42     10.942  73.766  47.995  1.00 12.99    B   C
ATOM  2333 CE  LYS B 42     12.343  73.611  47.372  1.00 12.98    B   C
ATOM  2334 NZ  LYS B 42     13.246  74.754  47.688  1.00 12.01    B   N
ATOM  2335 C   LYS B 42      6.273  71.981  47.593  1.00 19.30    B   C
ATOM  2336 O   LYS B 42      5.311  72.659  47.234  1.00 19.46    B   O
ATOM  2337 N   ASP B 43      6.206  71.042  48.526  1.00 19.11    B   N
ATOM  2338 CA  ASP B 43      4.903  70.766  49.089  1.00 20.39    B   C
ATOM  2339 CB  ASP B 43      4.970  69.389  49.727  1.00 26.23    B   C
ATOM  2340 CG  ASP B 43      3.668  68.908  50.218  1.00 34.18    B   C
ATOM  2341 OD1 ASP B 43      3.032  69.628  51.023  1.00 35.73    B   O
ATOM  2342 OD2 ASP B 43      3.286  67.802  49.834  1.00 34.67    B   O
ATOM  2343 C   ASP B 43      4.324  71.860  50.037  1.00 18.74    B   C
ATOM  2344 O   ASP B 43      5.067  72.590  50.662  1.00 17.52    B   O
ATOM  2345 N   PRO B 44      2.970  71.973  50.139  1.00 16.86    B   N
ATOM  2346 CD  PRO B 44      1.945  71.249  49.366  1.00 16.70    B   C
ATOM  2347 CA  PRO B 44      2.316  72.976  51.001  1.00 15.67    B   C
ATOM  2348 CB  PRO B 44      0.838  72.608  50.910  1.00 16.57    B   C
ATOM  2349 CG  PRO B 44      0.714  72.164  49.520  1.00 15.09    B   C
ATOM  2350 C   PRO B 44      2.785  73.063  52.460  1.00 14.32    B   C
ATOM  2351 O   PRO B 44      2.975  74.159  52.984  1.00 14.18    B   O
ATOM  2352 N   THR B 45      2.968  71.928  53.125  1.00 12.56    B   N
ATOM  2353 CA  THR B 45      3.404  71.976  54.513  1.00 15.07    B   C
ATOM  2354 CB  THR B 45      3.416  70.544  55.159  1.00 14.56    B   C
ATOM  2355 OG1 THR B 45      3.473  70.671  56.582  1.00 20.74    B   O
ATOM  2356 CG2 THR B 45      4.617  69.725  54.690  1.00 16.79    B   C
ATOM  2357 C   THR B 45      4.773  72.673  54.661  1.00 13.75    B   C
ATOM  2358 O   THR B 45      5.015  73.370  55.644  1.00 15.18    B   O
ATOM  2359 N   THR B 46      5.652  72.512  53.675  1.00 14.31    B   N
ATOM  2360 CA  THR B 46      6.978  73.138  53.708  1.00 13.76    B   C
ATOM  2361 CB  THR B 46      7.908  72.534  52.625  1.00 15.70    B   C
ATOM  2362 OG1 THR B 46      8.111  71.139  52.888  1.00 16.08    B   O
ATOM  2363 CG2 THR B 46      9.257  73.237  52.611  1.00 14.55    B   C
ATOM  2364 C   THR B 46      6.874  74.645  53.463  1.00 14.40    B   C
ATOM  2365 O   THR B 46      7.538  75.450  54.120  1.00 12.91    B   O
ATOM  2366 N   ILE B 47      6.029  75.016  52.509  1.00 12.98    B   N
ATOM  2367 CA  ILE B 47      5.843  76.414  52.159  1.00 14.06    B   C
ATOM  2368 CB  ILE B 47      4.987  76.537  50.881  1.00 12.60    B   C
ATOM  2369 CG2 ILE B 47      4.790  78.005  50.517  1.00 13.35    B   C
ATOM  2370 CG1 ILE B 47      5.684  75.804  49.727  1.00 14.48    B   C
ATOM  2371 CD1 ILE B 47      4.831  75.660  48.469  1.00 13.95    B   C
ATOM  2372 C   ILE B 47      5.193  77.190  53.305  1.00 13.29    B   C
ATOM  2373 O   ILE B 47      5.588  78.314  53.610  1.00 12.68    B   O
ATOM  2374 N   LYS B 48      4.199  76.594  53.948  1.00 13.12    B   N
ATOM  2375 CA  LYS B 48      3.541  77.279  55.047  1.00 14.82    B   C
ATOM  2376 CB  LYS B 48      2.387  76.440  55.606  1.00 15.61    B   C
ATOM  2377 CG  LYS B 48      1.239  76.283  54.621  1.00 16.82    B   C
ATOM  2378 CD  LYS B 48      0.021  75.649  55.261  1.00 17.71    B   C
ATOM  2379 CE  LYS B 48     -1.123  75.558  54.259  1.00 21.58    B   C
ATOM  2380 NZ  LYS B 48     -2.370  75.047  54.891  1.00 23.95    B   N
ATOM  2381 C   LYS B 48      4.537  77.600  56.145  1.00 15.64    B   C
ATOM  2382 O   LYS B 48      4.546  78.719  56.661  1.00 14.41    B   O
ATOM  2383 N   GLN B 49      5.383  76.630  56.493  1.00 13.94    B   N
ATOM  2384 CA  GLN B 49      6.388  76.836  57.533  1.00 14.63    B   C
ATOM  2385 CB  GLN B 49      7.127  75.520  57.822  1.00 15.57    B   C
ATOM  2386 CG  GLN B 49      8.185  75.577  58.930  1.00 19.33    B   C
ATOM  2387 CD  GLN B 49      7.656  76.099  60.258  1.00 18.82    B   C
ATOM  2388 OE1 GLN B 49      6.509  75.840  60.638  1.00 17.48    B   O
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Figure 6QQ

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ATOM  2389 NE2 GLN B 49     8.498 76.826 60.977 1.00 19.58    B   N
ATOM  2390 C   GLN B 49     7.357 77.934 57.091 1.00 15.00    B   C
ATOM  2391 O   GLN B 49     7.754 78.773 57.898 1.00 15.49    B   O
ATOM  2392 N   PHE B 50     7.732 77.936 55.812 1.00 13.73    B   N
ATOM  2393 CA  PHE B 50     8.617 78.978 55.297 1.00 12.73    B   C
ATOM  2394 CB  PHE B 50     8.813 78.845 53.784 1.00 12.69    B   C
ATOM  2395 CG  PHE B 50     9.756 77.740 53.372 1.00 14.11    B   C
ATOM  2396 CD1 PHE B 50    10.540 77.073 54.310 1.00 13.47    B   C
ATOM  2397 CD2 PHE B 50     9.884 77.396 52.028 1.00 16.97    B   C
ATOM  2398 CE1 PHE B 50    11.442 76.080 53.915 1.00 14.96    B   C
ATOM  2399 CE2 PHE B 50    10.784 76.405 51.622 1.00 16.26    B   C
ATOM  2400 CZ  PHE B 50    11.563 75.747 52.569 1.00 13.12    B   C
ATOM  2401 C   PHE B 50     7.999 80.348 55.586 1.00 12.88    B   C
ATOM  2402 O   PHE B 50     8.690 81.281 55.998 1.00 14.04    B   O
ATOM  2403 N   GLY B 51     6.692 80.460 55.353 1.00 13.99    B   N
ATOM  2404 CA  GLY B 51     5.992 81.712 55.590 1.00 13.72    B   C
ATOM  2405 C   GLY B 51     6.023 82.158 57.043 1.00 14.83    B   C
ATOM  2406 O   GLY B 51     6.243 83.334 57.331 1.00 11.98    B   O
ATOM  2407 N   LEU B 52     5.788 81.227 57.966 1.00 15.32    B   N
ATOM  2408 CA  LEU B 52     5.815 81.555 59.388 1.00 18.38    B   C
ATOM  2409 CB  LEU B 52     5.525 80.320 60.248 1.00 18.53    B   C
ATOM  2410 CG  LEU B 52     4.074 79.939 60.511 1.00 24.25    B   C
ATOM  2411 CD1 LEU B 52     3.349 79.724 59.198 1.00 27.80    B   C
ATOM  2412 CD2 LEU B 52     4.037 78.679 61.371 1.00 26.46    B   C
ATOM  2413 C   LEU B 52     7.184 82.091 59.757 1.00 18.61    B   C
ATOM  2414 O   LEU B 52     7.303 83.096 60.455 1.00 21.72    B   O
ATOM  2415 N   GLU B 53     8.219 81.404 59.289 1.00 18.50    B   N
ATOM  2416 CA  GLU B 53     9.584 81.811 59.573 1.00 17.94    B   C
ATOM  2417 CB  GLU B 53    10.551 80.751 59.038 1.00 17.42    B   C
ATOM  2418 CG  GLU B 53    10.566 79.507 59.927 1.00 15.49    B   C
ATOM  2419 CD  GLU B 53    11.305 78.332 59.323 1.00 17.96    B   C
ATOM  2420 OE1 GLU B 53    12.087 78.534 58.374 1.00 18.58    B   O
ATOM  2421 OE2 GLU B 53    11.105 77.201 59.813 1.00 19.70    B   O
ATOM  2422 C   GLU B 53     9.897 83.193 59.005 1.00 18.71    B   C
ATOM  2423 O   GLU B 53    10.680 83.945 59.579 1.00 19.86    B   O
ATOM  2424 N   ALA B 54     9.271 83.537 57.885 1.00 18.53    B   N
ATOM  2425 CA  ALA B 54     9.492 84.848 57.283 1.00 16.14    B   C
ATOM  2426 CB  ALA B 54     8.744 84.951 55.954 1.00 13.28    B   C
ATOM  2427 C   ALA B 54     9.009 85.934 58.257 1.00 18.34    B   C
ATOM  2428 O   ALA B 54     9.636 86.987 58.393 1.00 16.94    B   O
ATOM  2429 N   LEU B 55     7.898 85.669 58.941 1.00 17.14    B   N
ATOM  2430 CA  LEU B 55     7.361 86.629 59.901 1.00 18.57    B   C
ATOM  2431 CB  LEU B 55     6.118 86.060 60.594 1.00 19.89    B   C
ATOM  2432 CG  LEU B 55     4.827 85.855 59.795 1.00 20.72    B   C
ATOM  2433 CD1 LEU B 55     3.771 85.221 60.706 1.00 22.99    B   C
ATOM  2434 CD2 LEU B 55     4.321 87.192 59.251 1.00 23.42    B   C
ATOM  2435 C   LEU B 55     8.405 86.999 60.956 1.00 18.71    B   C
ATOM  2436 O   LEU B 55     8.555 88.170 61.301 1.00 17.21    B   O
ATOM  2437 N   ASP B 56     9.131 86.002 61.458 1.00 18.83    B   N
ATOM  2438 CA  ASP B 56    10.151 86.241 62.474 1.00 18.36    B   C
ATOM  2439 CB  ASP B 56    10.829 84.924 62.881 1.00 21.45    B   C
ATOM  2440 CG  ASP B 56     9.875 83.958 63.581 1.00 24.57    B   C
ATOM  2441 OD1 ASP B 56     9.003 84.419 64.344 1.00 27.38    B   O
ATOM  2442 OD2 ASP B 56    10.005 82.729 63.383 1.00 26.87    B   O
ATOM  2443 C   ASP B 56    11.211 87.240 62.014 1.00 19.11    B   C
ATOM  2444 O   ASP B 56    11.669 88.082 62.792 1.00 17.72    B   O
ATOM  2445 N   PHE B 57    11.598 87.154 60.746 1.00 17.66    B   N
ATOM  2446 CA  PHE B 57    12.607 88.063 60.216 1.00 16.52    B   C
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Figure 6RR

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ATOM  2447  CB  PHE B  57      12.867  87.794  58.732  1.00 16.73      B   C
ATOM  2448  CG  PHE B  57      13.656  88.879  58.071  1.00 17.10      B   C
ATOM  2449  CD1 PHE B  57      15.035  88.958  58.247  1.00 19.76      B   C
ATOM  2450  CD2 PHE B  57      13.010  89.889  57.366  1.00 14.93      B   C
ATOM  2451  CE1 PHE B  57      15.759  90.031  57.738  1.00 19.78      B   C
ATOM  2452  CE2 PHE B  57      13.721  90.966  56.854  1.00 19.53      B   C
ATOM  2453  CZ  PHE B  57      15.100  91.039  57.041  1.00 19.60      B   C
ATOM  2454  C   PHE B  57      12.222  89.529  60.360  1.00 16.52      B   C
ATOM  2455  O   PHE B  57      13.057  90.365  60.699  1.00 18.03      B   O
ATOM  2456  N   PHE B  58      10.962  89.842  60.082  1.00 15.91      B   N
ATOM  2457  CA  PHE B  58      10.497  91.222  60.144  1.00 18.80      B   C
ATOM  2458  CB  PHE B  58       9.233  91.385  59.295  1.00 17.22      B   C
ATOM  2459  CG  PHE B  58       9.465  91.219  57.825  1.00 18.15      B   C
ATOM  2460  CD1 PHE B  58       9.217  90.004  57.199  1.00 18.00      B   C
ATOM  2461  CD2 PHE B  58       9.927  92.283  57.061  1.00 17.52      B   C
ATOM  2462  CE1 PHE B  58       9.423  89.852  55.831  1.00 16.31      B   C
ATOM  2463  CE2 PHE B  58      10.136  92.142  55.694  1.00 16.57      B   C
ATOM  2464  CZ  PHE B  58       9.884  90.924  55.077  1.00 17.04      B   C
ATOM  2465  C   PHE B  58      10.224  91.809  61.522  1.00 18.66      B   C
ATOM  2466  O   PHE B  58      10.140  93.028  61.662  1.00 21.14      B   O
ATOM  2467  N   LYS B  59      10.080  90.958  62.531  1.00 19.45      B   N
ATOM  2468  CA  LYS B  59       9.769  91.429  63.877  1.00 21.34      B   C
ATOM  2469  CB  LYS B  59       9.816  90.258  64.858  1.00 22.87      B   C
ATOM  2470  CG  LYS B  59       8.740  89.213  64.571  1.00 27.48      B   C
ATOM  2471  CD  LYS B  59       8.762  88.088  65.585  1.00 28.84      B   C
ATOM  2472  CE  LYS B  59       7.612  87.121  65.345  1.00 32.72      B   C
ATOM  2473  NZ  LYS B  59       6.308  87.829  65.430  1.00 35.68      B   N
ATOM  2474  C   LYS B  59      10.614  92.596  64.384  1.00 20.43      B   C
ATOM  2475  O   LYS B  59      10.073  93.621  64.792  1.00 19.96      B   O
ATOM  2476  N   PRO B  60      11.948  92.468  64.356  1.00 20.32      B   N
ATOM  2477  CD  PRO B  60      12.784  91.337  63.911  1.00 19.12      B   C
ATOM  2478  CA  PRO B  60      12.776  93.579  64.837  1.00 19.99      B   C
ATOM  2479  CB  PRO B  60      14.181  92.980  64.848  1.00 21.24      B   C
ATOM  2480  CG  PRO B  60      14.131  91.991  63.719  1.00 22.69      B   C
ATOM  2481  C   PRO B  60      12.690  94.859  63.995  1.00 20.53      B   C
ATOM  2482  O   PRO B  60      13.030  95.943  64.472  1.00 18.48      B   O
ATOM  2483  N   HIS B  61      12.221  94.740  62.756  1.00 18.92      B   N
ATOM  2484  CA  HIS B  61      12.116  95.896  61.871  1.00 20.35      B   C
ATOM  2485  CB  HIS B  61      12.099  95.433  60.413  1.00 19.99      B   C
ATOM  2486  CG  HIS B  61      13.409  94.875  59.953  1.00 19.89      B   C
ATOM  2487  CD2 HIS B  61      13.820  93.599  59.768  1.00 21.62      B   C
ATOM  2488  ND1 HIS B  61      14.499  95.673  59.678  1.00 21.05      B   N
ATOM  2489  CE1 HIS B  61      15.526  94.912  59.343  1.00 22.27      B   C
ATOM  2490  NE2 HIS B  61      15.142  93.649  59.390  1.00 21.05      B   N
ATOM  2491  C   HIS B  61      10.904  96.770  62.170  1.00 21.73      B   C
ATOM  2492  O   HIS B  61      10.808  97.899  61.691  1.00 22.05      B   O
ATOM  2493  N   GLU B  62       9.985  96.242  62.969  1.00 21.87      B   N
ATOM  2494  CA  GLU B  62       8.792  96.982  63.354  1.00 23.56      B   C
ATOM  2495  CB  GLU B  62       9.181  98.106  64.318  1.00 24.92      B   C
ATOM  2496  CG  GLU B  62      10.003  97.606  65.496  1.00 30.01      B   C
ATOM  2497  CD  GLU B  62      10.361  98.699  66.481  1.00 33.69      B   C
ATOM  2498  OE1 GLU B  62      10.896  99.743  66.053  1.00 35.60      B   O
ATOM  2499  OE2 GLU B  62      10.116  98.505  67.688  1.00 36.17      B   O
ATOM  2500  C   GLU B  62       8.044  97.552  62.157  1.00 22.92      B   C
ATOM  2501  O   GLU B  62       7.701  98.739  62.126  1.00 21.97      B   O
ATOM  2502  N   ILE B  63       7.795  96.706  61.164  1.00 19.69      B   N
ATOM  2503  CA  ILE B  63       7.064  97.144  59.987  1.00 18.17      B   C
ATOM  2504  CB  ILE B  63       7.236  96.149  58.825  1.00 17.22      B   C
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Figure 6SS

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ATOM  2505 CG2 ILE B  63      8.686  96.146  58.370  1.00 15.56    B   C
ATOM  2506 CG1 ILE B  63      6.817  94.746  59.269  1.00 15.21    B   C
ATOM  2507 CD1 ILE B  63.     6.745  93.736  58.131  1.00 15.19    B   C
ATOM  2508 C   ILE B  63      5.590  97.258  60.375  1.00 18.21    B   C
ATOM  2509 O   ILE B  63      5.127  96.575  61.294  1.00 17.53    B   O
ATOM  2510 N   GLU B  64      4.859  98.125  59.683  1.00 16.97    B   N
ATOM  2511 CA  GLU B  64      3.445  98.349  59.985  1.00 17.61    B   C
ATOM  2512 CB  GLU B  64      3.089  99.813  59.718  1.00 18.92    B   C
ATOM  2513 CG  GLU B  64      3.934 100.801  60.499  1.00 23.07    B   C
ATOM  2514 CD  GLU B  64      3.697 102.235  60.067  1.00 26.42    B   C
ATOM  2515 OE1 GLU B  64      2.541 102.702  60.167  1.00 28.70    B   O
ATOM  2516 OE2 GLU B  64      4.667 102.889  59.624  1.00 25.35    B   O
ATOM  2517 C   GLU B  64      2.511  97.452  59.187  1.00 16.83    B   C
ATOM  2518 O   GLU B  64      1.349  97.259  59.548  1.00 16.07    B   O
ATOM  2519 N   LEU B  65      3.035  96.896  58.104  1.00 17.77    B   N
ATOM  2520 CA  LEU B  65      2.261  96.031  57.232  1.00 16.43    B   C
ATOM  2521 CB  LEU B  65      1.398  96.895  56.302  1.00 18.09    B   C
ATOM  2522 CG  LEU B  65      0.640  96.266  55.133  1.00 21.97    B   C
ATOM  2523 CD1 LEU B  65     -0.529  97.164  54.757  1.00 21.04    B   C
ATOM  2524 CD2 LEU B  65      1.572  96.066  53.944  1.00 20.71    B   C
ATOM  2525 C   LEU B  65      3.244  95.195  56.430  1.00 14.51    B   C
ATOM  2526 O   LEU B  65      4.345  95.648  56.123  1.00 12.92    B   O
ATOM  2527 N   LEU B  66      2.853  93.971  56.102  1.00 14.75    B   N
ATOM  2528 CA  LEU B  66      3.722  93.092  55.329  1.00 14.89    B   C
ATOM  2529 CB  LEU B  66      4.020  91.810  56.110  1.00 14.10    B   C
ATOM  2530 CG  LEU B  66      4.753  90.716  55.326  1.00 16.87    B   C
ATOM  2531 CD1 LEU B  66      6.149  91.214  54.949  1.00 16.67    B   C
ATOM  2532 CD2 LEU B  66      4.844  89.433  56.169  1.00 17.63    B   C
ATOM  2533 C   LEU B  66      3.091  92.722  53.995  1.00 14.55    B   C
ATOM  2534 O   LEU B  66      1.911  92.374  53.923  1.00 16.90    B   O
ATOM  2535 N   ILE B  67      3.884  92.813  52.937  1.00 14.59    B   N
ATOM  2536 CA  ILE B  67      3.422  92.451  51.610  1.00 14.92    B   C
ATOM  2537 CB  ILE B  67      3.775  93.524  50.560  1.00 17.24    B   C
ATOM  2538 CG2 ILE B  67      3.458  93.000  49.150  1.00 14.44    B   C
ATOM  2539 CG1 ILE B  67      2.995  94.815  50.846  1.00 17.41    B   C
ATOM  2540 CD1 ILE B  67      3.287  95.933  49.859  1.00 18.39    B   C
ATOM  2541 C   ILE B  67      4.117  91.159  51.207  1.00 13.22    B   C
ATOM  2542 O   ILE B  67      5.344  91.077  51.219  1.00 13.66    B   O
ATOM  2543 N   VAL B  68      3.330  90.144  50.875  1.00 13.61    B   N
ATOM  2544 CA  VAL B  68      3.898  88.878  50.430  1.00 13.77    B   C
ATOM  2545 CB  VAL B  68      3.065  87.683  50.915  1.00 12.35    B   C
ATOM  2546 CG1 VAL B  68      3.692  86.381  50.426  1.00 10.26    B   C
ATOM  2547 CG2 VAL B  68      2.991  87.699  52.438  1.00 12.86    B   C
ATOM  2548 C   VAL B  68      3.865  88.950  48.907  1.00 12.64    B   C
ATOM  2549 O   VAL B  68      2.839  88.673  48.283  1.00 14.77    B   O
ATOM  2550 N   ALA B  69      4.988  89.349  48.319  1.00 12.26    B   N
ATOM  2551 CA  ALA B  69      5.101  89.499  46.870  1.00 10.06    B   C
ATOM  2552 CB  ALA B  69      6.412  90.194  46.529  1.00  9.84    B   C
ATOM  2553 C   ALA B  69      5.027  88.163  46.147  1.00 12.35    B   C
ATOM  2554 O   ALA B  69      4.635  88.096  44.980  1.00  9.71    B   O
ATOM  2555 N   CYS B  70      5.427  87.104  46.844  1.00 11.11    B   N
ATOM  2556 CA  CYS B  70      5.418  85.766  46.273  1.00 11.24    B   C
ATOM  2557 CB  CYS B  70      6.207  84.816  47.176  1.00 11.62    B   C
ATOM  2558 SG  CYS B  70      6.347  83.142  46.504  1.00 12.64    B   S
ATOM  2559 C   CYS B  70      4.001  85.229  46.070  1.00 11.05    B   C
ATOM  2560 O   CYS B  70      3.205  85.177  47.010  1.00 11.37    B   O
ATOM  2561 N   ASN B  71      3.688  84.823  44.840  1.00 12.49    B   N
ATOM  2562 CA  ASN B  71      2.365  84.279  44.543  1.00 11.50    B   C
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Figure 6TT

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ATOM  2563  CB  ASN B  71      2.157  84.145  43.031  1.00  9.14      B   C
ATOM  2564  CG  ASN B  71      2.258  85.471  42.306  1.00 11.76      B   C
ATOM  2565  OD1 ASN B  71      3.344  86.024  42.151  1.00 10.78      B   O
ATOM  2566  ND2 ASN B  71      1.117  85.996  41.867  1.00 11.54      B   N
ATOM  2567  C   ASN B  71      2.192  82.909  45.186  1.00 12.35      B   C
ATOM  2568  O   ASN B  71      1.078  82.526  45.575  1.00  8.22      B   O
ATOM  2569  N   THR B  72      3.292  82.164  45.270  1.00 11.41      B   N
ATOM  2570  CA  THR B  72      3.257  80.831  45.863  1.00 12.16      B   C
ATOM  2571  CB  THR B  72      4.572  80.062  45.611  1.00 13.52      B   C
ATOM  2572  OG1 THR B  72      4.704  79.791  44.212  1.00 14.69      B   O
ATOM  2573  CG2 THR B  72      4.581  78.741  46.380  1.00 11.87      B   C
ATOM  2574  C   THR B  72      3.012  80.915  47.357  1.00 12.59      B   C
ATOM  2575  O   THR B  72      2.166  80.200  47.892  1.00 14.73      B   O
ATOM  2576  N   ALA B  73      3.754  81.784  48.034  1.00 13.02      B   N
ATOM  2577  CA  ALA B  73      3.576  81.953  49.471  1.00 13.51      B   C
ATOM  2578  CB  ALA B  73      4.676  82.830  50.044  1.00 13.14      B   C
ATOM  2579  C   ALA B  73      2.206  82.571  49.739  1.00 13.74      B   C
ATOM  2580  O   ALA B  73      1.580  82.278  50.752  1.00 12.89      B   O
ATOM  2581  N   SER B  74      1.751  83.437  48.830  1.00 14.66      B   N
ATOM  2582  CA  SER B  74      0.439  84.066  48.967  1.00 14.25      B   C
ATOM  2583  CB  SER B  74      0.212  85.099  47.853  1.00 13.54      B   C
ATOM  2584  OG  SER B  74      0.996  86.268  48.040  1.00 13.45      B   O
ATOM  2585  C   SER B  74     -0.655  83.002  48.877  1.00 16.32      B   C
ATOM  2586  O   SER B  74     -1.668  83.065  49.575  1.00 14.08      B   O
ATOM  2587  N   ALA B  75     -0.443  82.028  48.002  1.00 16.22      B   N
ATOM  2588  CA  ALA B  75     -1.416  80.966  47.797  1.00 17.85      B   C
ATOM  2589  CB  ALA B  75     -1.170  80.291  46.449  1.00 18.98      B   C
ATOM  2590  C   ALA B  75     -1.438  79.911  48.890  1.00 18.56      B   C
ATOM  2591  O   ALA B  75     -2.498  79.377  49.217  1.00 19.22      B   O
ATOM  2592  N   LEU B  76     -0.274  79.608  49.455  1.00 17.86      B   N
ATOM  2593  CA  LEU B  76     -0.196  78.570  50.473  1.00 19.90      B   C
ATOM  2594  CB  LEU B  76      0.921  77.580  50.131  1.00 19.60      B   C
ATOM  2595  CG  LEU B  76      0.703  76.565  49.004  1.00 21.94      B   C
ATOM  2596  CD1 LEU B  76     -0.579  75.764  49.283  1.00 19.11      B   C
ATOM  2597  CD2 LEU B  76      0.610  77.284  47.670  1.00 23.22      B   C
ATOM  2598  C   LEU B  76     -0.021  78.978  51.925  1.00 19.97      B   C
ATOM  2599  O   LEU B  76     -0.643  78.388  52.800  1.00 19.54      B   O
ATOM  2600  N   ALA B  77      0.815  79.980  52.183  1.00 20.55      B   N
ATOM  2601  CA  ALA B  77      1.111  80.380  53.559  1.00 22.00      B   C
ATOM  2602  CB  ALA B  77      2.616  80.581  53.700  1.00 20.40      B   C
ATOM  2603  C   ALA B  77      0.392  81.590  54.149  1.00 21.97      B   C
ATOM  2604  O   ALA B  77      0.420  81.792  55.365  1.00 17.66      B   O
ATOM  2605  N   LEU B  78     -0.247  82.386  53.299  1.00 23.46      B   N
ATOM  2606  CA  LEU B  78     -0.916  83.595  53.757  1.00 24.17      B   C
ATOM  2607  CB  LEU B  78     -1.634  84.271  52.583  1.00 23.46      B   C
ATOM  2608  CG  LEU B  78     -2.166  85.692  52.799  1.00 24.62      B   C
ATOM  2609  CD1 LEU B  78     -1.042  86.612  53.256  1.00 25.18      B   C
ATOM  2610  CD2 LEU B  78     -2.770  86.204  51.499  1.00 21.11      B   C
ATOM  2611  C   LEU B  78     -1.885  83.387  54.918  1.00 23.63      B   C
ATOM  2612  O   LEU B  78     -1.820  84.098  55.918  1.00 20.90      B   O
ATOM  2613  N   GLU B  79     -2.775  82.410  54.798  1.00 24.20      B   N
ATOM  2614  CA  GLU B  79     -3.744  82.171  55.856  1.00 25.27      B   C
ATOM  2615  CB  GLU B  79     -4.643  80.987  55.496  1.00 27.94      B   C
ATOM  2616  CG  GLU B  79     -5.845  80.830  56.417  1.00 34.09      B   C
ATOM  2617  CD  GLU B  79     -6.760  79.694  55.997  1.00 36.98      B   C
ATOM  2618  OE1 GLU B  79     -7.246  79.714  54.847  1.00 38.97      B   O
ATOM  2619  OE2 GLU B  79     -6.994  78.781  56.818  1.00 40.71      B   O
ATOM  2620  C   GLU B  79     -3.066  81.921  57.199  1.00 24.66      B   C
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Figure 6UU

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ATOM  2621 O   GLU B 79    -3.434  82.519  58.208  1.00 21.76    B   O
ATOM  2622 N   GLU B 80    -2.063  81.050  57.213  1.00 25.11    B   N
ATOM  2623 CA  GLU B 80    -1.367  80.740  58.455  1.00 25.16    B   C
ATOM  2624 CB  GLU B 80    -0.425  79.549  58.249  1.00 30.59    B   C
ATOM  2625 CG  GLU B 80    -0.324  78.632  59.464  1.00 36.68    B   C
ATOM  2626 CD  GLU B 80    -1.674  78.055  59.876  1.00 39.61    B   C
ATOM  2627 OE1 GLU B 80    -2.275  77.297  59.085  1.00 42.54    B   O
ATOM  2628 OE2 GLU B 80    -2.139  78.363  60.993  1.00 41.38    B   O
ATOM  2629 C   GLU B 80    -0.587  81.942  58.987  1.00 24.73    B   C
ATOM  2630 O   GLU B 80    -0.590  82.211  60.190  1.00 24.93    B   O
ATOM  2631 N   MET B 81     0.072  82.670  58.092  1.00 22.49    B   N
ATOM  2632 CA  MET B 81     0.851  83.838  58.492  1.00 20.82    B   C
ATOM  2633 CB  MET B 81     1.559  84.437  57.275  1.00 18.38    B   C
ATOM  2634 CG  MET B 81     2.671  83.563  56.717  1.00 18.17    B   C
ATOM  2635 SD  MET B 81     3.255  84.147  55.112  1.00 17.68    B   S
ATOM  2636 CE  MET B 81     4.308  85.481  55.573  1.00 12.45    B   C
ATOM  2637 C   MET B 81    -0.015  84.907  59.155  1.00 20.81    B   C
ATOM  2638 O   MET B 81     0.382  85.508  60.154  1.00 19.23    B   O
ATOM  2639 N   GLN B 82    -1.193  85.145  58.589  1.00 20.82    B   N
ATOM  2640 CA  GLN B 82    -2.111  86.145  59.129  1.00 22.97    B   C
ATOM  2641 CB  GLN B 82    -3.286  86.367  58.168  1.00 23.14    B   C
ATOM  2642 CG  GLN B 82    -2.861  86.867  56.787  1.00 22.68    B   C
ATOM  2643 CD  GLN B 82    -4.024  87.016  55.821  1.00 25.48    B   C
ATOM  2644 OE1 GLN B 82    -4.830  86.097  55.650  1.00 24.87    B   O
ATOM  2645 NE2 GLN B 82    -4.110  88.175  55.172  1.00 25.37    B   N
ATOM  2646 C   GLN B 82    -2.627  85.695  60.482  1.00 22.69    B   C
ATOM  2647 O   GLN B 82    -2.905  86.514  61.357  1.00 22.32    B   O
ATOM  2648 N   LYS B 83    -2.752  84.387  60.656  1.00 24.09    B   N
ATOM  2649 CA  LYS B 83    -3.235  83.851  61.918  1.00 25.60    B   C
ATOM  2650 CB  LYS B 83    -3.376  82.328  61.829  1.00 27.86    B   C
ATOM  2651 CG  LYS B 83    -3.766  81.658  63.141  1.00 32.07    B   C
ATOM  2652 CD  LYS B 83    -3.799  80.148  62.990  1.00 33.64    B   C
ATOM  2653 CE  LYS B 83    -4.118  79.453  64.308  1.00 38.06    B   C
ATOM  2654 NZ  LYS B 83    -4.127  77.965  64.142  1.00 38.15    B   N
ATOM  2655 C   LYS B 83    -2.298  84.218  63.065  1.00 25.66    B   C
ATOM  2656 O   LYS B 83    -2.750  84.586  64.149  1.00 23.94    B   O
ATOM  2657 N   TYR B 84    -0.993  84.134  62.825  1.00 25.08    B   N
ATOM  2658 CA  TYR B 84    -0.022  84.442  63.870  1.00 24.54    B   C
ATOM  2659 CB  TYR B 84     1.063  83.367  63.913  1.00 27.22    B   C
ATOM  2660 CG  TYR B 84     0.542  81.986  64.219  1.00 30.76    B   C
ATOM  2661 CD1 TYR B 84     0.162  81.119  63.195  1.00 31.28    B   C
ATOM  2662 CE1 TYR B 84    -0.325  79.844  63.476  1.00 34.59    B   C
ATOM  2663 CD2 TYR B 84     0.421  81.546  65.538  1.00 32.96    B   C
ATOM  2664 CE2 TYR B 84    -0.066  80.276  65.832  1.00 35.61    B   C
ATOM  2665 CZ  TYR B 84    -0.435  79.430  64.797  1.00 36.06    B   C
ATOM  2666 OH  TYR B 84    -0.904  78.167  65.089  1.00 37.33    B   O
ATOM  2667 C   TYR B 84     0.641  85.808  63.764  1.00 23.89    B   C
ATOM  2668 O   TYR B 84     1.704  86.030  64.341  1.00 25.50    B   O
ATOM  2669 N   SER B 85     0.014  86.726  63.040  1.00 22.10    B   N
ATOM  2670 CA  SER B 85     0.563  88.067  62.874  1.00 21.74    B   C
ATOM  2671 CB  SER B 85     0.884  88.323  61.397  1.00 19.79    B   C
ATOM  2672 OG  SER B 85     1.259  89.673  61.181  1.00 25.60    B   O
ATOM  2673 C   SER B 85    -0.413  89.127  63.374  1.00 21.62    B   C
ATOM  2674 O   SER B 85    -1.621  89.009  63.177  1.00 21.34    B   O
ATOM  2675 N   LYS B 86     0.107  90.157  64.031  1.00 20.33    B   N
ATOM  2676 CA  LYS B 86    -0.750  91.221  64.519  1.00 22.30    B   C
ATOM  2677 CB  LYS B 86    -0.235  91.776  65.853  1.00 25.37    B   C
ATOM  2678 CG  LYS B 86     1.182  92.304  65.826  1.00 31.07    B   C
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Figure 6VV

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ATOM  2679 CD  LYS B  86      1.629  92.685  67.231  1.00 35.40      B   C
ATOM  2680 CE  LYS B  86      1.562  91.486  68.175  1.00 35.66      B   C
ATOM  2681 NZ  LYS B  86      1.952  91.849  69.565  1.00 39.76      B   N
ATOM  2682 C   LYS B  86     -0.860  92.333  63.482  1.00 22.13      B   C
ATOM  2683 O   LYS B  86     -1.871  93.028  63.433  1.00 23.41      B   O
ATOM  2684 N   ILE B  87      0.169  92.499  62.649  1.00 20.24      B   N
ATOM  2685 CA  ILE B  87      0.127  93.524  61.605  1.00 18.31      B   C
ATOM  2686 CB  ILE B  87      1.543  94.004  61.181  1.00 16.92      B   C
ATOM  2687 CG2 ILE B  87      2.244  94.688  62.359  1.00 18.70      B   C
ATOM  2688 CG1 ILE B  87      2.361  92.822  60.650  1.00 17.63      B   C
ATOM  2689 CD1 ILE B  87      3.721  93.203  60.117  1.00 17.00      B   C
ATOM  2690 C   ILE B  87     -0.559  92.921  60.384  1.00 17.72      B   C
ATOM  2691 O   ILE B  87     -0.553  91.707  60.193  1.00 18.08      B   O
ATOM  2692 N   PRO B  88     -1.173  93.762  59.542  1.00 18.77      B   N
ATOM  2693 CD  PRO B  88     -1.340  95.223  59.619  1.00 17.15      B   C
ATOM  2694 CA  PRO B  88     -1.839  93.216  58.358  1.00 19.35      B   C
ATOM  2695 CB  PRO B  88     -2.575  94.428  57.789  1.00 20.10      B   C
ATOM  2696 CG  PRO B  88     -1.691  95.572  58.194  1.00 21.95      B   C
ATOM  2697 C   PRO B  88     -0.844  92.619  57.360  1.00 18.71      B   C
ATOM  2698 O   PRO B  88      0.247  93.148  57.163  1.00 18.85      B   O
ATOM  2699 N   ILE B  89     -1.222  91.498  56.759  1.00 17.91      B   N
ATOM  2700 CA  ILE B  89     -0.387  90.848  55.757  1.00 17.91      B   C
ATOM  2701 CB  ILE B  89     -0.011  89.404  56.164  1.00 18.44      B   C
ATOM  2702 CG2 ILE B  89      0.952  88.807  55.133  1.00 18.14      B   C
ATOM  2703 CG1 ILE B  89      0.658  89.408  57.543  1.00 21.01      B   C
ATOM  2704 CD1 ILE B  89      1.125  88.043  58.007  1.00 18.58      B   C
ATOM  2705 C   ILE B  89     -1.202  90.823  54.466  1.00 17.23      B   C
ATOM  2706 O   ILE B  89     -2.323  90.305  54.425  1.00 17.75      B   O
ATOM  2707 N   VAL B  90     -0.642  91.403  53.414  1.00 16.10      B   N
ATOM  2708 CA  VAL B  90     -1.334  91.467  52.141  1.00 15.66      B   C
ATOM  2709 CB  VAL B  90     -1.436  92.934  51.651  1.00 17.82      B   C
ATOM  2710 CG1 VAL B  90     -2.241  93.001  50.351  1.00 17.58      B   C
ATOM  2711 CG2 VAL B  90     -2.074  93.805  52.739  1.00 18.13      B   C
ATOM  2712 C   VAL B  90     -0.612  90.640  51.088  1.00 13.43      B   C
ATOM  2713 O   VAL B  90      0.567  90.869  50.812  1.00 14.69      B   O
ATOM  2714 N   GLY B  91     -1.332  89.681  50.511  1.00 13.52      B   N
ATOM  2715 CA  GLY B  91     -0.773  88.827  49.474  1.00 12.39      B   C
ATOM  2716 C   GLY B  91     -1.085  89.387  48.093  1.00 14.87      B   C
ATOM  2717 O   GLY B  91     -1.754  90.414  47.982  1.00 13.52      B   O
ATOM  2718 N   VAL B  92     -0.618  88.715  47.041  1.00 13.75      B   N
ATOM  2719 CA  VAL B  92     -0.840  89.190  45.676  1.00 14.98      B   C
ATOM  2720 CB  VAL B  92      0.447  89.066  44.819  1.00 14.03      B   C
ATOM  2721 CG1 VAL B  92      1.442  90.130  45.234  1.00  9.89      B   C
ATOM  2722 CG2 VAL B  92      1.056  87.672  44.978  1.00 12.60      B   C
ATOM  2723 C   VAL B  92     -1.975  88.505  44.922  1.00 16.65      B   C
ATOM  2724 O   VAL B  92     -2.194  88.786  43.746  1.00 17.87      B   O
ATOM  2725 N   ILE B  93     -2.702  87.616  45.585  1.00 16.90      B   N
ATOM  2726 CA  ILE B  93     -3.798  86.933  44.909  1.00 17.60      B   C
ATOM  2727 CB  ILE B  93     -3.993  85.514  45.469  1.00 18.08      B   C
ATOM  2728 CG2 ILE B  93     -5.148  84.825  44.757  1.00 15.25      B   C
ATOM  2729 CG1 ILE B  93     -2.693  84.722  45.291  1.00 18.10      B   C
ATOM  2730 CD1 ILE B  93     -2.803  83.256  45.609  1.00 20.71      B   C
ATOM  2731 C   ILE B  93     -5.125  87.693  44.971  1.00 18.37      B   C
ATOM  2732 O   ILE B  93     -5.720  87.983  43.930  1.00 19.27      B   O
ATOM  2733 N   GLU B  94     -5.590  88.021  46.176  1.00 18.78      B   N
ATOM  2734 CA  GLU B  94     -6.859  88.742  46.315  1.00 21.11      B   C
ATOM  2735 CB  GLU B  94     -7.198  88.977  47.789  1.00 23.95      B   C
ATOM  2736 CG  GLU B  94     -7.565  87.705  48.536  1.00 28.58      B   C
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Figure 6WW

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ATOM  2737 CD  GLU B  94     -8.651  86.906  47.831  1.00 33.34    B   C
ATOM  2738 OE1 GLU B  94     -9.700  87.494  47.484  1.00 32.87    B   O
ATOM  2739 OE2 GLU B  94     -8.453  85.686  47.627  1.00 36.08    B   O
ATOM  2740 C   GLU B  94     -6.873  90.073  45.568  1.00 20.94    B   C
ATOM  2741 O   GLU B  94     -7.882  90.439  44.960  1.00 21.06    B   O
ATOM  2742 N   PRO B  95     -5.760  90.823  45.615  1.00 19.29    B   N
ATOM  2743 CD  PRO B  95     -4.581  90.667  46.487  1.00 17.34    B   C
ATOM  2744 CA  PRO B  95     -5.714  92.108  44.909  1.00 19.84    B   C
ATOM  2745 CB  PRO B  95     -4.301  92.603  45.196  1.00 18.81    B   C
ATOM  2746 CG  PRO B  95     -4.058  92.087  46.580  1.00 19.00    B   C
ATOM  2747 C   PRO B  95     -5.971  91.933  43.415  1.00 18.63    B   C
ATOM  2748 O   PRO B  95     -6.588  92.786  42.771  1.00 19.30    B   O
ATOM  2749 N   SER B  96     -5.485  90.824  42.867  1.00 20.23    B   N
ATOM  2750 CA  SER B  96     -5.661  90.532  41.451  1.00 19.54    B   C
ATOM  2751 CB  SER B  96     -4.752  89.380  41.032  1.00 20.19    B   C
ATOM  2752 OG  SER B  96     -3.398  89.803  41.022  1.00 21.10    B   O
ATOM  2753 C   SER B  96     -7.107  90.194  41.137  1.00 19.82    B   C
ATOM  2754 O   SER B  96     -7.623  90.554  40.076  1.00 18.36    B   O
ATOM  2755 N   ILE B  97     -7.761  89.496  42.060  1.00 19.40    B   N
ATOM  2756 CA  ILE B  97     -9.159  89.129  41.869  1.00 21.46    B   C
ATOM  2757 CB  ILE B  97     -9.702  88.310  43.066  1.00 20.75    B   C
ATOM  2758 CG2 ILE B  97    -11.185  88.032  42.872  1.00 23.74    B   C
ATOM  2759 CG1 ILE B  97     -8.929  86.996  43.205  1.00 20.33    B   C
ATOM  2760 CD1 ILE B  97     -9.130  86.028  42.048  1.00 18.39    B   C
ATOM  2761 C   ILE B  97     -9.985  90.408  41.741  1.00 20.42    B   C
ATOM  2762 O   ILE B  97    -10.881  90.502  40.904  1.00 21.88    B   O
ATOM  2763 N   LEU B  98     -9.670  91.393  42.575  1.00 22.89    B   N
ATOM  2764 CA  LEU B  98    -10.378  92.668  42.561  1.00 22.94    B   C
ATOM  2765 CB  LEU B  98     -9.918  93.539  43.734  1.00 24.42    B   C
ATOM  2766 CG  LEU B  98    -10.197  92.998  45.143  1.00 24.87    B   C
ATOM  2767 CD1 LEU B  98     -9.532  93.893  46.172  1.00 27.53    B   C
ATOM  2768 CD2 LEU B  98    -11.701  92.922  45.389  1.00 25.92    B   C
ATOM  2769 C   LEU B  98    -10.150  93.411  41.249  1.00 23.55    B   C
ATOM  2770 O   LEU B  98    -11.067  94.032  40.708  1.00 24.17    B   O
ATOM  2771 N   ALA B  99     -8.924  93.351  40.740  1.00 23.11    B   N
ATOM  2772 CA  ALA B  99     -8.594  94.025  39.491  1.00 22.89    B   C
ATOM  2773 CB  ALA B  99     -7.110  93.904  39.208  1.00 22.27    B   C
ATOM  2774 C   ALA B  99     -9.390  93.395  38.362  1.00 21.70    B   C
ATOM  2775 O   ALA B  99     -9.921  94.090  37.497  1.00 18.65    B   O
ATOM  2776 N   ILE B 100     -9.457  92.068  38.377  1.00 19.64    B   N
ATOM  2777 CA  ILE B 100    -10.190  91.331  37.363  1.00 19.82    B   C
ATOM  2778 CB  ILE B 100    -10.044  89.803  37.568  1.00 21.33    B   C
ATOM  2779 CG2 ILE B 100    -11.118  89.054  36.784  1.00 19.75    B   C
ATOM  2780 CG1 ILE B 100     -8.644  89.357  37.134  1.00 20.47    B   C
ATOM  2781 CD1 ILE B 100     -8.425  87.859  37.227  1.00 23.03    B   C
ATOM  2782 C   ILE B 100    -11.664  91.717  37.413  1.00 20.18    B   C
ATOM  2783 O   ILE B 100    -12.310  91.842  36.378  1.00 17.92    B   O
ATOM  2784 N   LYS B 101    -12.192  91.910  38.617  1.00 21.96    B   N
ATOM  2785 CA  LYS B 101    -13.594  92.296  38.755  1.00 24.71    B   C
ATOM  2786 CB  LYS B 101    -13.980  92.434  40.229  1.00 25.47    B   C
ATOM  2787 CG  LYS B 101    -14.034  91.120  40.988  1.00 30.47    B   C
ATOM  2788 CD  LYS B 101    -14.348  91.358  42.460  1.00 36.47    B   C
ATOM  2789 CE  LYS B 101    -15.720  91.992  42.654  1.00 39.30    B   C
ATOM  2790 NZ  LYS B 101    -15.973  92.336  44.087  1.00 42.89    B   N
ATOM  2791 C   LYS B 101    -13.831  93.623  38.041  1.00 24.26    B   C
ATOM  2792 O   LYS B 101    -14.846  93.797  37.369  1.00 25.28    B   O
ATOM  2793 N   ARG B 102    -12.886  94.548  38.185  1.00 23.53    B   N
ATOM  2794 CA  ARG B 102    -12.986  95.865  37.559  1.00 24.45    B   C
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Figure 6XX

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ATOM  2795 CB  ARG B 102   -11.976  96.835  38.182  1.00 24.23    B   C
ATOM  2796 CG  ARG B 102   -12.234  97.217  39.625  1.00 25.40    B   C
ATOM  2797 CD  ARG B 102   -11.276  98.316  40.054  1.00 26.37    B   C
ATOM  2798 NE  ARG B 102    -9.888  97.863  40.086  1.00 27.81    B   N
ATOM  2799 CZ  ARG B 102    -9.328  97.229  41.114  1.00 27.91    B   C
ATOM  2800 NH1 ARG B 102   -10.035  96.972  42.206  1.00 27.77    B   N
ATOM  2801 NH2 ARG B 102    -8.058  96.857  41.051  1.00 22.49    B   N
ATOM  2802 C   ARG B 102   -12.747  95.846  36.051  1.00 23.56    B   C
ATOM  2803 O   ARG B 102   -13.394  96.576  35.306  1.00 21.65    B   O
ATOM  2804 N   GLN B 103   -11.816  95.010  35.605  1.00 22.46    B   N
ATOM  2805 CA  GLN B 103   -11.474  94.951  34.189  1.00 22.58    B   C
ATOM  2806 CB  GLN B 103    -9.972  94.728  34.036  1.00 21.32    B   C
ATOM  2807 CG  GLN B 103    -9.126  95.766  34.733  1.00 22.61    B   C
ATOM  2808 CD  GLN B 103    -7.659  95.405  34.712  1.00 22.94    B   C
ATOM  2809 OE1 GLN B 103    -7.074  95.216  33.647  1.00 24.42    B   O
ATOM  2810 NE2 GLN B 103    -7.055  95.305  35.890  1.00 22.74    B   N
ATOM  2811 C   GLN B 103   -12.206  93.918  33.349  1.00 22.98    B   C
ATOM  2812 O   GLN B 103   -12.221  94.020  32.126  1.00 23.73    B   O
ATOM  2813 N   VAL B 104   -12.807  92.925  33.989  1.00 22.89    B   N
ATOM  2814 CA  VAL B 104   -13.500  91.881  33.241  1.00 24.65    B   C
ATOM  2815 CB  VAL B 104   -12.796  90.518  33.427  1.00 25.96    B   C
ATOM  2816 CG1 VAL B 104   -13.465  89.462  32.568  1.00 25.99    B   C
ATOM  2817 CG2 VAL B 104   -11.321  90.643  33.066  1.00 24.05    B   C
ATOM  2818 C   VAL B 104   -14.957  91.752  33.663  1.00 26.14    B   C
ATOM  2819 O   VAL B 104   -15.284  90.975  34.557  1.00 23.04    B   O
ATOM  2820 N   GLU B 105   -15.821  92.515  33.000  1.00 28.13    B   N
ATOM  2821 CA  GLU B 105   -17.253  92.520  33.289  1.00 31.78    B   C
ATOM  2822 CB  GLU B 105   -17.923  93.703  32.581  1.00 37.19    B   C
ATOM  2823 CG  GLU B 105   -17.318  95.053  32.940  1.00 47.02    B   C
ATOM  2824 CD  GLU B 105   -17.983  96.226  32.231  1.00 50.74    B   C
ATOM  2825 OE1 GLU B 105   -18.016  96.247  30.979  1.00 51.99    B   O
ATOM  2826 OE2 GLU B 105   -18.469  97.136  32.933  1.00 54.70    B   O
ATOM  2827 C   GLU B 105   -17.953  91.231  32.877  1.00 29.48    B   C
ATOM  2828 O   GLU B 105   -18.915  90.807  33.518  1.00 32.30    B   O
ATOM  2829 N   ASP B 106   -17.471  90.608  31.808  1.00 27.12    B   N
ATOM  2830 CA  ASP B 106   -18.067  89.377  31.310  1.00 26.01    B   C
ATOM  2831 CB  ASP B 106   -17.666  89.167  29.850  1.00 26.98    B   C
ATOM  2832 CG  ASP B 106   -18.215  87.881  29.272  1.00 28.23    B   C
ATOM  2833 OD1 ASP B 106   -19.054  87.232  29.930  1.00 28.83    B   O
ATOM  2834 OD2 ASP B 106   -17.807  87.521  28.147  1.00 31.85    B   O
ATOM  2835 C   ASP B 106   -17.666  88.168  32.147  1.00 25.85    B   C
ATOM  2836 O   ASP B 106   -16.517  87.736  32.118  1.00 24.84    B   O
ATOM  2837 N   LYS B 107   -18.628  87.626  32.890  1.00 25.49    B   N
ATOM  2838 CA  LYS B 107   -18.396  86.472  33.754  1.00 27.31    B   C
ATOM  2839 CB  LYS B 107   -19.633  86.210  34.622  1.00 29.26    B   C
ATOM  2840 CG  LYS B 107   -19.948  87.328  35.600  1.00 32.01    B   C
ATOM  2841 CD  LYS B 107   -18.757  87.611  36.512  1.00 33.91    B   C
ATOM  2842 CE  LYS B 107   -19.056  88.718  37.516  1.00 34.29    B   C
ATOM  2843 NZ  LYS B 107   -19.369  90.016  36.853  1.00 41.19    B   N
ATOM  2844 C   LYS B 107   -18.044  85.203  32.991  1.00 26.67    B   C
ATOM  2845 O   LYS B 107   -17.508  84.254  33.565  1.00 28.78    B   O
ATOM  2846 N   ASN B 108   -18.337  85.187  31.698  1.00 26.36    B   N
ATOM  2847 CA  ASN B 108   -18.059  84.019  30.875  1.00 27.30    B   C
ATOM  2848 CB  ASN B 108   -19.176  83.833  29.848  1.00 32.21    B   C
ATOM  2849 CG  ASN B 108   -20.509  83.515  30.496  1.00 37.21    B   C
ATOM  2850 OD1 ASN B 108   -20.670  82.470  31.130  1.00 41.66    B   O
ATOM  2851 ND2 ASN B 108   -21.473  84.420  30.350  1.00 39.88    B   N
ATOM  2852 C   ASN B 108   -16.719  84.106  30.160  1.00 25.00    B   C
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Figure 6YY

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ATOM  2853  O   ASN B 108    -16.318  83.173  29.467  1.00 27.12      B   O
ATOM  2854  N   ALA B 109    -16.029  85.227  30.333  1.00 22.44      B   N
ATOM  2855  CA  ALA B 109    -14.734  85.427  29.696  1.00 22.32      B   C
ATOM  2856  CB  ALA B 109    -14.179  86.795  30.062  1.00 19.60      B   C
ATOM  2857  C   ALA B 109    -13.768  84.334  30.133  1.00 21.09      B   C
ATOM  2858  O   ALA B 109    -13.580  84.107  31.326  1.00 21.33      B   O
ATOM  2859  N   PRO B 110    -13.152  83.635  29.168  1.00 21.10      B   N
ATOM  2860  CD  PRO B 110    -13.315  83.775  27.711  1.00 21.88      B   C
ATOM  2861  CA  PRO B 110    -12.201  82.562  29.485  1.00 21.55      B   C
ATOM  2862  CB  PRO B 110    -11.843  81.988  28.111  1.00 20.46      B   C
ATOM  2863  CG  PRO B 110    -13.002  82.387  27.233  1.00 23.31      B   C
ATOM  2864  C   PRO B 110    -10.974  83.142  30.190  1.00 21.39      B   C
ATOM  2865  O   PRO B 110    -10.243  83.950  29.615  1.00 20.23      B   O
ATOM  2866  N   ILE B 111    -10.757  82.731  31.433  1.00 20.74      B   N
ATOM  2867  CA  ILE B 111     -9.621  83.220  32.208  1.00 21.29      B   C
ATOM  2868  CB  ILE B 111    -10.085  83.770  33.575  1.00 18.70      B   C
ATOM  2869  CG2 ILE B 111     -8.883  84.214  34.398  1.00 19.35      B   C
ATOM  2870  CG1 ILE B 111    -11.054  84.937  33.365  1.00 17.87      B   C
ATOM  2871  CD1 ILE B 111    -11.768  85.374  34.632  1.00 13.74      B   C
ATOM  2872  C   ILE B 111     -8.618  82.096  32.439  1.00 20.50      B   C
ATOM  2873  O   ILE B 111     -8.983  81.017  32.900  1.00 21.37      B   O
ATOM  2874  N   LEU B 112     -7.358  82.354  32.107  1.00 19.57      B   N
ATOM  2875  CA  LEU B 112     -6.302  81.367  32.285  1.00 18.55      B   C
ATOM  2876  CB  LEU B 112     -5.538  81.154  30.975  1.00 17.95      B   C
ATOM  2877  CG  LEU B 112     -4.340  80.200  31.024  1.00 18.08      B   C
ATOM  2878  CD1 LEU B 112     -4.774  78.812  31.482  1.00 19.26      B   C
ATOM  2879  CD2 LEU B 112     -3.713  80.132  29.640  1.00 16.52      B   C
ATOM  2880  C   LEU B 112     -5.329  81.799  33.370  1.00 18.08      B   C
ATOM  2881  O   LEU B 112     -4.731  82.873  33.291  1.00 19.20      B   O
ATOM  2882  N   VAL B 113     -5.171  80.951  34.380  1.00 16.92      B   N
ATOM  2883  CA  VAL B 113     -4.269  81.231  35.487  1.00 16.68      B   C
ATOM  2884  CB  VAL B 113     -4.863  80.728  36.835  1.00 17.69      B   C
ATOM  2885  CG1 VAL B 113     -3.945  81.110  37.994  1.00 17.55      B   C
ATOM  2886  CG2 VAL B 113     -6.244  81.309  37.050  1.00 17.01      B   C
ATOM  2887  C   VAL B 113     -2.943  80.516  35.243  1.00 16.02      B   C
ATOM  2888  O   VAL B 113     -2.921  79.308  34.999  1.00 14.64      B   O
ATOM  2889  N   LEU B 114     -1.845  81.267  35.291  1.00 14.63      B   N
ATOM  2890  CA  LEU B 114     -0.520  80.692  35.104  1.00 13.92      B   C
ATOM  2891  CB  LEU B 114      0.247  81.395  33.979  1.00 11.65      B   C
ATOM  2892  CG  LEU B 114     -0.330  81.466  32.566  1.00 17.67      B   C
ATOM  2893  CD1 LEU B 114      0.736  82.064  31.644  1.00 16.72      B   C
ATOM  2894  CD2 LEU B 114     -0.738  80.081  32.077  1.00 17.71      B   C
ATOM  2895  C   LEU B 114      0.256  80.881  36.399  1.00 14.25      B   C
ATOM  2896  O   LEU B 114      0.210  81.947  37.005  1.00 11.47      B   O
ATOM  2897  N   GLY B 115      0.984  79.855  36.813  1.00 14.70      B   N
ATOM  2898  CA  GLY B 115      1.757  79.971  38.037  1.00 15.73      B   C
ATOM  2899  C   GLY B 115      2.608  78.746  38.289  1.00 14.74      B   C
ATOM  2900  O   GLY B 115      2.693  77.855  37.451  1.00 13.78      B   O
ATOM  2901  N   THR B 116      3.252  78.706  39.447  1.00 16.02      B   N
ATOM  2902  CA  THR B 116      4.087  77.568  39.798  1.00 15.11      B   C
ATOM  2903  CB  THR B 116      4.916  77.860  41.045  1.00 14.07      B   C
ATOM  2904  OG1 THR B 116      4.040  78.104  42.155  1.00 12.96      B   O
ATOM  2905  CG2 THR B 116      5.800  79.074  40.814  1.00 13.81      B   C
ATOM  2906  C   THR B 116      3.182  76.375  40.083  1.00 15.15      B   C
ATOM  2907  O   THR B 116      1.974  76.528  40.260  1.00 15.43      B   O
ATOM  2908  N   LYS B 117      3.768  75.189  40.124  1.00 14.92      B   N
ATOM  2909  CA  LYS B 117      2.998  73.991  40.401  1.00 16.68      B   C
ATOM  2910  CB  LYS B 117      3.926  72.776  40.462  1.00 18.20      B   C
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Figure 6ZZ

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ATOM  2911 CG  LYS B 117      3.170  71.459  40.516  1.00 28.15      B   C
ATOM  2912 CD  LYS B 117      2.286  71.334  39.280  1.00 34.68      B   C
ATOM  2913 CE  LYS B 117      1.422  70.089  39.310  1.00 37.95      B   C
ATOM  2914 NZ  LYS B 117      0.628  69.995  38.057  1.00 40.68      B   N
ATOM  2915 C   LYS B 117      2.231  74.125  41.725  1.00 15.54      B   C
ATOM  2916 O   LYS B 117      1.055  73.772  41.811  1.00 13.25      B   O
ATOM  2917 N   ALA B 118      2.896  74.648  42.753  1.00 13.55      B   N
ATOM  2918 CA  ALA B 118      2.263  74.797  44.062  1.00 13.07      B   C
ATOM  2919 CB  ALA B 118      3.294  75.271  45.092  1.00 13.77      B   C
ATOM  2920 C   ALA B 118      1.084  75.755  44.020  1.00 13.96      B   C
ATOM  2921 O   ALA B 118      0.022  75.478  44.584  1.00 12.32      B   O
ATOM  2922 N   THR B 119      1.270  76.887  43.347  1.00 12.40      B   N
ATOM  2923 CA  THR B 119      0.204  77.874  43.248  1.00 14.50      B   C
ATOM  2924 CB  THR B 119      0.698  79.159  42.534  1.00 11.89      B   C
ATOM  2925 OG1 THR B 119      1.739  79.763  43.311  1.00 13.56      B   O
ATOM  2926 CG2 THR B 119     -0.443  80.158  42.373  1.00 12.19      B   C
ATOM  2927 C   THR B 119     -1.005  77.312  42.504  1.00 12.61      B   C
ATOM  2928 O   THR B 119     -2.140  77.473  42.942  1.00 15.20      B   O
ATOM  2929 N   ILE B 120     -0.759  76.641  41.385  1.00 13.07      B   N
ATOM  2930 CA  ILE B 120     -1.847  76.080  40.594  1.00 17.11      B   C
ATOM  2931 CB  ILE B 120     -1.333  75.521  39.242  1.00 15.75      B   C
ATOM  2932 CG2 ILE B 120     -2.499  74.993  38.418  1.00 19.67      B   C
ATOM  2933 CG1 ILE B 120     -0.600  76.620  38.461  1.00 15.38      B   C
ATOM  2934 CD1 ILE B 120     -1.456  77.829  38.120  1.00 19.05      B   C
ATOM  2935 C   ILE B 120     -2.605  74.971  41.331  1.00 17.21      B   C
ATOM  2936 O   ILE B 120     -3.832  74.938  41.309  1.00 18.55      B   O
ATOM  2937 N   GLN B 121     -1.887  74.064  41.984  1.00 17.85      B   N
ATOM  2938 CA  GLN B 121     -2.554  72.983  42.700  1.00 21.02      B   C
ATOM  2939 CB  GLN B 121     -1.539  71.946  43.177  1.00 23.26      B   C
ATOM  2940 CG  GLN B 121     -0.796  71.267  42.053  1.00 31.27      B   C
ATOM  2941 CD  GLN B 121     -0.046  70.038  42.509  1.00 34.42      B   C
ATOM  2942 OE1 GLN B 121      0.702  70.078  43.488  1.00 38.77      B   O
ATOM  2943 NE2 GLN B 121     -0.237  68.933  41.797  1.00 36.80      B   N
ATOM  2944 C   GLN B 121     -3.375  73.477  43.894  1.00 21.84      B   C
ATOM  2945 O   GLN B 121     -4.297  72.795  44.345  1.00 23.51      B   O
ATOM  2946 N   SER B 122     -3.056  74.661  44.404  1.00 20.44      B   N
ATOM  2947 CA  SER B 122     -3.791  75.193  45.549  1.00 20.89      B   C
ATOM  2948 CB  SER B 122     -3.024  76.348  46.208  1.00 20.03      B   C
ATOM  2949 OG  SER B 122     -3.115  77.537  45.438  1.00 19.77      B   O
ATOM  2950 C   SER B 122     -5.178  75.687  45.152  1.00 19.13      B   C
ATOM  2951 O   SER B 122     -6.057  75.812  46.000  1.00 18.67      B   O
ATOM  2952 N   ASN B 123     -5.362  75.960  43.864  1.00 20.34      B   N
ATOM  2953 CA  ASN B 123     -6.626  76.476  43.345  1.00 21.65      B   C
ATOM  2954 CB  ASN B 123     -7.756  75.464  43.543  1.00 24.19      B   C
ATOM  2955 CG  ASN B 123     -7.662  74.302  42.583  1.00 28.22      B   C
ATOM  2956 OD1 ASN B 123     -7.618  74.492  41.368  1.00 28.03      B   O
ATOM  2957 ND2 ASN B 123     -7.632  73.087  43.121  1.00 31.95      B   N
ATOM  2958 C   ASN B 123     -6.990  77.787  44.025  1.00 20.93      B   C
ATOM  2959 O   ASN B 123     -8.162  78.160  44.098  1.00 20.81      B   O
ATOM  2960 N   ALA B 124     -5.977  78.488  44.520  1.00 18.37      B   N
ATOM  2961 CA  ALA B 124     -6.205  79.759  45.187  1.00 19.77      B   C
ATOM  2962 CB  ALA B 124     -4.872  80.387  45.588  1.00 18.94      B   C
ATOM  2963 C   ALA B 124     -6.993  80.715  44.285  1.00 18.40      B   C
ATOM  2964 O   ALA B 124     -8.032  81.239  44.685  1.00 20.72      B   O
ATOM  2965 N   TYR B 125     -6.506  80.936  43.069  1.00 19.24      B   N
ATOM  2966 CA  TYR B 125     -7.184  81.841  42.142  1.00 19.32      B   C
ATOM  2967 CB  TYR B 125     -6.331  82.091  40.892  1.00 19.37      B   C
ATOM  2968 CG  TYR B 125     -5.129  82.989  41.102  1.00 19.31      B   C
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Figure 6AAA

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ATOM  2969 CD1 TYR B 125     -3.887  82.457  41.439  1.00 17.61    B   C
ATOM  2970 CE1 TYR B 125     -2.768  83.280  41.591  1.00 18.62    B   C
ATOM  2971 CD2 TYR B 125     -5.228  84.371  40.929  1.00 17.15    B   C
ATOM  2972 CE2 TYR B 125     -4.123  85.197  41.078  1.00 16.64    B   C
ATOM  2973 CZ  TYR B 125     -2.895  84.646  41.405  1.00 17.43    B   C
ATOM  2974 OH  TYR B 125     -1.792  85.454  41.520  1.00 17.10    B   O
ATOM  2975 C   TYR B 125     -8.553  81.340  41.696  1.00 19.25    B   C
ATOM  2976 O   TYR B 125     -9.528  82.096  41.688  1.00 18.74    B   O
ATOM  2977 N   ASP B 126     -8.617  80.071  41.310  1.00 18.47    B   N
ATOM  2978 CA  ASP B 126     -9.862  79.473  40.841  1.00 19.68    B   C
ATOM  2979 CB  ASP B 126     -9.660  77.986  40.552  1.00 19.72    B   C
ATOM  2980 CG  ASP B 126     -8.455  77.720  39.671  1.00 23.51    B   C
ATOM  2981 OD1 ASP B 126     -7.341  78.138  40.042  1.00 24.96    B   O
ATOM  2982 OD2 ASP B 126     -8.621  77.085  38.609  1.00 22.93    B   O
ATOM  2983 C   ASP B 126    -10.972  79.635  41.868  1.00 21.84    B   C
ATOM  2984 O   ASP B 126    -12.076  80.077  41.541  1.00 18.17    B   O
ATOM  2985 N   ASN B 127    -10.676  79.273  43.113  1.00 21.58    B   N
ATOM  2986 CA  ASN B 127    -11.659  79.376  44.181  1.00 22.68    B   C
ATOM  2987 CB  ASN B 127    -11.081  78.839  45.495  1.00 22.98    B   C
ATOM  2988 CG  ASN B 127    -10.656  77.385  45.393  1.00 26.68    B   C
ATOM  2989 OD1 ASN B 127    -11.290  76.591  44.701  1.00 26.92    B   O
ATOM  2990 ND2 ASN B 127     -9.582  77.029  46.092  1.00 29.75    B   N
ATOM  2991 C   ASN B 127    -12.105  80.821  44.362  1.00 22.20    B   C
ATOM  2992 O   ASN B 127    -13.300  81.104  44.443  1.00 22.96    B   O
ATOM  2993 N   ALA B 128    -11.145  81.736  44.422  1.00 21.77    B   N
ATOM  2994 CA  ALA B 128    -11.465  83.149  44.587  1.00 22.81    B   C
ATOM  2995 CB  ALA B 128    -10.184  83.970  44.693  1.00 24.04    B   C
ATOM  2996 C   ALA B 128    -12.315  83.643  43.422  1.00 24.10    B   C
ATOM  2997 O   ALA B 128    -13.302  84.354  43.624  1.00 27.04    B   O
ATOM  2998 N   LEU B 129    -11.935  83.262  42.205  1.00 24.54    B   N
ATOM  2999 CA  LEU B 129    -12.672  83.664  41.012  1.00 24.58    B   C
ATOM  3000 CB  LEU B 129    -11.926  83.225  39.753  1.00 22.03    B   C
ATOM  3001 CG  LEU B 129    -10.633  83.975  39.418  1.00 24.03    B   C
ATOM  3002 CD1 LEU B 129     -9.865  83.210  38.366  1.00 22.36    B   C
ATOM  3003 CD2 LEU B 129    -10.956  85.382  38.932  1.00 22.58    B   C
ATOM  3004 C   LEU B 129    -14.078  83.070  41.005  1.00 26.08    B   C
ATOM  3005 O   LEU B 129    -15.046  83.751  40.669  1.00 26.16    B   O
ATOM  3006 N   LYS B 130    -14.185  81.795  41.365  1.00 26.80    B   N
ATOM  3007 CA  LYS B 130    -15.482  81.130  41.404  1.00 29.37    B   C
ATOM  3008 CB  LYS B 130    -15.326  79.694  41.904  1.00 32.59    B   C
ATOM  3009 CG  LYS B 130    -16.638  78.939  42.019  1.00 37.42    B   C
ATOM  3010 CD  LYS B 130    -17.337  78.877  40.675  1.00 43.42    B   C
ATOM  3011 CE  LYS B 130    -18.708  78.237  40.775  1.00 45.02    B   C
ATOM  3012 NZ  LYS B 130    -19.379  78.220  39.444  1.00 49.29    B   N
ATOM  3013 C   LYS B 130    -16.400  81.897  42.347  1.00 29.56    B   C
ATOM  3014 O   LYS B 130    -17.538  82.218  42.010  1.00 28.29    B   O
ATOM  3015 N   GLN B 131    -15.876  82.185  43.532  1.00 29.31    B   N
ATOM  3016 CA  GLN B 131    -16.599  82.911  44.559  1.00 31.88    B   C
ATOM  3017 CB  GLN B 131    -15.667  83.162  45.747  1.00 35.97    B   C
ATOM  3018 CG  GLN B 131    -16.286  83.913  46.918  1.00 45.23    B   C
ATOM  3019 CD  GLN B 131    -17.385  83.128  47.610  1.00 50.61    B   C
ATOM  3020 OE1 GLN B 131    -17.211  81.951  47.942  1.00 53.57    B   O
ATOM  3021 NE2 GLN B 131    -18.524  83.781  47.843  1.00 52.00    B   N
ATOM  3022 C   GLN B 131    -17.137  84.239  44.035  1.00 31.40    B   C
ATOM  3023 O   GLN B 131    -18.222  84.675  44.427  1.00 29.81    B   O
ATOM  3024 N   GLN B 132    -16.382  84.878  43.145  1.00 29.49    B   N
ATOM  3025 CA  GLN B 132    -16.788  86.166  42.597  1.00 29.13    B   C
ATOM  3026 CB  GLN B 132    -15.558  87.020  42.290  1.00 30.78    B   C
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Figure 6BBB

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ATOM  3027  CG  GLN B 132    -14.776  87.410  43.535  1.00 32.44    B   C
ATOM  3028  CD  GLN B 132    -15.644  88.114  44.565  1.00 35.76    B   C
ATOM  3029  OE1 GLN B 132    -16.234  89.158  44.286  1.00 35.79    B   O
ATOM  3030  NE2 GLN B 132    -15.725  87.542  45.763  1.00 34.46    B   N
ATOM  3031  C   GLN B 132    -17.682  86.079  41.368  1.00 29.17    B   C
ATOM  3032  O   GLN B 132    -17.994  87.096  40.747  1.00 28.85    B   O
ATOM  3033  N   GLY B 133    -18.075  84.864  41.004  1.00 28.71    B   N
ATOM  3034  CA  GLY B 133    -18.974  84.700  39.879  1.00 28.15    B   C
ATOM  3035  C   GLY B 133    -18.442  84.343  38.509  1.00 27.61    B   C
ATOM  3036  O   GLY B 133    -19.224  84.310  37.561  1.00 26.00    B   O
ATOM  3037  N   TYR B 134    -17.146  84.078  38.371  1.00 26.83    B   N
ATOM  3038  CA  TYR B 134    -16.627  83.721  37.056  1.00 26.16    B   C
ATOM  3039  CB  TYR B 134    -15.135  84.049  36.961  1.00 24.55    B   C
ATOM  3040  CG  TYR B 134    -14.921  85.545  36.938  1.00 22.77    B   C
ATOM  3041  CD1 TYR B 134    -14.840  86.277  38.123  1.00 22.62    B   C
ATOM  3042  CE1 TYR B 134    -14.760  87.670  38.109  1.00 23.49    B   C
ATOM  3043  CD2 TYR B 134    -14.911  86.246  35.730  1.00 24.51    B   C
ATOM  3044  CE2 TYR B 134    -14.834  87.641  35.702  1.00 25.08    B   C
ATOM  3045  CZ  TYR B 134    -14.759  88.346  36.896  1.00 23.66    B   C
ATOM  3046  OH  TYR B 134    -14.689  89.721  36.886  1.00 24.39    B   O
ATOM  3047  C   TYR B 134    -16.927  82.264  36.729  1.00 26.95    B   C
ATOM  3048  O   TYR B 134    -16.774  81.379  37.571  1.00 26.50    B   O
ATOM  3049  N   LEU B 135    -17.362  82.031  35.494  1.00 25.91    B   N
ATOM  3050  CA  LEU B 135    -17.777  80.704  35.049  1.00 28.31    B   C
ATOM  3051  CB  LEU B 135    -19.155  80.822  34.388  1.00 28.49    B   C
ATOM  3052  CG  LEU B 135    -20.131  81.733  35.139  1.00 28.21    B   C
ATOM  3053  CD1 LEU B 135    -21.343  82.031  34.272  1.00 28.13    B   C
ATOM  3054  CD2 LEU B 135    -20.527  81.077  36.455  1.00 29.07    B   C
ATOM  3055  C   LEU B 135    -16.847  79.940  34.113  1.00 27.36    B   C
ATOM  3056  O   LEU B 135    -17.066  78.758  33.855  1.00 27.87    B   O
ATOM  3057  N   ASN B 136    -15.819  80.602  33.596  1.00 28.12    B   N
ATOM  3058  CA  ASN B 136    -14.892  79.944  32.681  1.00 25.99    B   C
ATOM  3059  CB  ASN B 136    -15.053  80.520  31.276  1.00 27.18    B   C
ATOM  3060  CG  ASN B 136    -14.416  79.652  30.214  1.00 27.92    B   C
ATOM  3061  OD1 ASN B 136    -13.572  78.807  30.509  1.00 28.48    B   O
ATOM  3062  ND2 ASN B 136    -14.809  79.866  28.962  1.00 30.11    B   N
ATOM  3063  C   ASN B 136    -13.460  80.159  33.172  1.00 26.03    B   C
ATOM  3064  O   ASN B 136    -12.749  81.040  32.688  1.00 24.61    B   O
ATOM  3065  N   ILE B 137    -13.046  79.342  34.133  1.00 24.40    B   N
ATOM  3066  CA  ILE B 137    -11.715  79.451  34.716  1.00 24.19    B   C
ATOM  3067  CB  ILE B 137    -11.816  79.575  36.254  1.00 25.00    B   C
ATOM  3068  CG2 ILE B 137    -10.430  79.802  36.857  1.00 26.36    B   C
ATOM  3069  CG1 ILE B 137    -12.752  80.735  36.616  1.00 25.12    B   C
ATOM  3070  CD1 ILE B 137    -13.231  80.738  38.056  1.00 25.56    B   C
ATOM  3071  C   ILE B 137    -10.809  78.268  34.378  1.00 24.30    B   C
ATOM  3072  O   ILE B 137    -11.180  77.114  34.574  1.00 24.24    B   O
ATOM  3073  N   SER B 138     -9.620  78.570  33.865  1.00 22.99    B   N
ATOM  3074  CA  SER B 138     -8.640  77.545  33.520  1.00 23.07    B   C
ATOM  3075  CB  SER B 138     -8.357  77.547  32.016  1.00 21.90    B   C
ATOM  3076  OG  SER B 138     -9.532  77.297  31.271  1.00 28.80    B   O
ATOM  3077  C   SER B 138     -7.345  77.845  34.267  1.00 21.12    B   C
ATOM  3078  O   SER B 138     -7.104  78.986  34.675  1.00 18.88    B   O
ATOM  3079  N   HIS B 139     -6.521  76.820  34.463  1.00 20.44    B   N
ATOM  3080  CA  HIS B 139     -5.242  77.010  35.134  1.00 20.66    B   C
ATOM  3081  CB  HIS B 139     -5.343  76.712  36.639  1.00 20.23    B   C
ATOM  3082  CG  HIS B 139     -5.802  75.322  36.964  1.00 21.50    B   C
ATOM  3083  CD2 HIS B 139     -5.241  74.114  36.716  1.00 22.63    B   C
ATOM  3084  ND1 HIS B 139     -6.984  75.067  37.626  1.00 20.86    B   N
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Figure 6CCC

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ATOM  3085 CE1 HIS B 139     -7.132  73.761  37.770  1.00 23.65    B   C
ATOM  3086 NE2 HIS B 139     -6.089  73.161  37.226  1.00 23.23    B   N
ATOM  3087 C   HIS B 139     -4.172  76.148  34.488  1.00 21.34    B   C
ATOM  3088 O   HIS B 139     -4.468  75.120  33.874  1.00 21.81    B   O
ATOM  3089 N   LEU B 140     -2.922  76.578  34.614  1.00 21.36    B   N
ATOM  3090 CA  LEU B 140     -1.815  75.846  34.023  1.00 20.20    B   C
ATOM  3091 CB  LEU B 140     -1.644  76.244  32.558  1.00 21.19    B   C
ATOM  3092 CG  LEU B 140     -0.502  75.564  31.800  1.00 21.50    B   C
ATOM  3093 CD1 LEU B 140     -0.790  74.074  31.688  1.00 21.95    B   C
ATOM  3094 CD2 LEU B 140     -0.357  76.190  30.410  1.00 21.96    B   C
ATOM  3095 C   LEU B 140     -0.511  76.104  34.758  1.00 19.11    B   C
ATOM  3096 O   LEU B 140     -0.098  77.248  34.928  1.00 16.59    B   O
ATOM  3097 N   ALA B 141      0.135  75.027  35.186  1.00 19.36    B   N
ATOM  3098 CA  ALA B 141      1.405  75.133  35.887  1.00 19.87    B   C
ATOM  3099 CB  ALA B 141      1.603  73.918  36.791  1.00 21.48    B   C
ATOM  3100 C   ALA B 141      2.531  75.215  34.856  1.00 16.62    B   C
ATOM  3101 O   ALA B 141      2.912  74.214  34.261  1.00 20.61    B   O
ATOM  3102 N   THR B 142      3.049  76.415  34.630  1.00 15.84    B   N
ATOM  3103 CA  THR B 142      4.132  76.600  33.676  1.00 14.20    B   C
ATOM  3104 CB  THR B 142      3.948  77.913  32.889  1.00 13.97    B   C
ATOM  3105 OG1 THR B 142      3.814  79.003  33.806  1.00 14.25    B   O
ATOM  3106 CG2 THR B 142      2.691  77.840  32.023  1.00 13.62    B   C
ATOM  3107 C   THR B 142      5.410  76.652  34.505  1.00 14.37    B   C
ATOM  3108 O   THR B 142      6.114  77.653  34.529  1.00 13.97    B   O
ATOM  3109 N   SER B 143      5.698  75.544  35.176  1.00 15.59    B   N
ATOM  3110 CA  SER B 143      6.844  75.444  36.067  1.00 16.89    B   C
ATOM  3111 CB  SER B 143      6.971  74.013  36.591  1.00 19.31    B   C
ATOM  3112 OG  SER B 143      8.003  73.931  37.564  1.00 27.09    B   O
ATOM  3113 C   SER B 143      8.193  75.902  35.537  1.00 16.21    B   C
ATOM  3114 O   SER B 143      8.892  76.666  36.205  1.00 16.07    B   O
ATOM  3115 N   LEU B 144      8.557  75.446  34.345  1.00 15.08    B   N
ATOM  3116 CA  LEU B 144      9.850  75.783  33.759  1.00 15.48    B   C
ATOM  3117 CB  LEU B 144     10.094  74.929  32.520  1.00 15.32    B   C
ATOM  3118 CG  LEU B 144     10.215  73.436  32.827  1.00 16.70    B   C
ATOM  3119 CD1 LEU B 144     10.267  72.642  31.536  1.00 19.80    B   C
ATOM  3120 CD2 LEU B 144     11.468  73.190  33.654  1.00 19.07    B   C
ATOM  3121 C   LEU B 144     10.037  77.251  33.421  1.00 14.68    B   C
ATOM  3122 O   LEU B 144     11.145  77.678  33.098  1.00 14.35    B   O
ATOM  3123 N   PHE B 145      8.962  78.028  33.484  1.00 14.12    B   N
ATOM  3124 CA  PHE B 145      9.088  79.447  33.199  1.00 15.35    B   C
ATOM  3125 CB  PHE B 145      7.719  80.148  33.232  1.00 13.56    B   C
ATOM  3126 CG  PHE B 145      6.911  79.992  31.964  1.00 14.58    B   C
ATOM  3127 CD1 PHE B 145      5.657  80.594  31.852  1.00 13.83    B   C
ATOM  3128 CD2 PHE B 145      7.393  79.252  30.888  1.00 16.08    B   C
ATOM  3129 CE1 PHE B 145      4.899  80.461  30.688  1.00 14.15    B   C
ATOM  3130 CE2 PHE B 145      6.646  79.111  29.720  1.00 15.95    B   C
ATOM  3131 CZ  PHE B 145      5.395  79.717  29.620  1.00 14.39    B   C
ATOM  3132 C   PHE B 145     10.011  80.084  34.233  1.00 14.15    B   C
ATOM  3133 O   PHE B 145     10.821  80.942  33.896  1.00 13.84    B   O
ATOM  3134 N   VAL B 146      9.901  79.648  35.488  1.00 14.43    B   N
ATOM  3135 CA  VAL B 146     10.721  80.215  36.558  1.00 15.36    B   C
ATOM  3136 CB  VAL B 146     10.353  79.617  37.949  1.00 17.29    B   C
ATOM  3137 CG1 VAL B 146     11.367  80.065  38.995  1.00 16.50    B   C
ATOM  3138 CG2 VAL B 146      8.959  80.079  38.369  1.00 14.60    B   C
ATOM  3139 C   VAL B 146     12.229  80.086  36.329  1.00 14.39    B   C
ATOM  3140 O   VAL B 146     12.935  81.092  36.326  1.00 14.20    B   O
ATOM  3141 N   PRO B 147     12.747  78.856  36.144  1.00 14.14    B   N
ATOM  3142 CD  PRO B 147     12.141  77.519  36.269  1.00 13.43    B   C
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Figure 6DDD

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ATOM  3143 CA  PRO B 147     14.195  78.754  35.921  1.00 14.59      B   C
ATOM  3144 CB  PRO B 147     14.457  77.242  35.995  1.00 13.53      B   C
ATOM  3145 CG  PRO B 147     13.151  76.642  35.573  1.00 14.07      B   C
ATOM  3146 C   PRO B 147     14.653  79.377  34.597  1.00 13.40      B   C
ATOM  3147 O   PRO B 147     15.775  79.877  34.500  1.00 13.19      B   O
ATOM  3148 N   LEU B 148     13.796  79.355  33.577  1.00 11.38      B   N
ATOM  3149 CA  LEU B 148     14.179  79.960  32.303  1.00 12.63      B   C
ATOM  3150 CB  LEU B 148     13.100  79.751  31.232  1.00 14.70      B   C
ATOM  3151 CG  LEU B 148     13.404  78.655  30.202  1.00 12.09      B   C
ATOM  3152 CD1 LEU B 148     13.446  77.315  30.903  1.00 14.46      B   C
ATOM  3153 CD2 LEU B 148     12.341  78.649  29.106  1.00 18.20      B   C
ATOM  3154 C   LEU B 148     14.395  81.448  32.508  1.00 12.91      B   C
ATOM  3155 O   LEU B 148     15.372  82.018  32.031  1.00 12.96      B   O
ATOM  3156 N   ILE B 149     13.471  82.070  33.231  1.00 13.00      B   N
ATOM  3157 CA  ILE B 149     13.545  83.500  33.499  1.00 12.87      B   C
ATOM  3158 CB  ILE B 149     12.211  83.989  34.130  1.00 13.86      B   C
ATOM  3159 CG2 ILE B 149     12.352  85.419  34.647  1.00 12.28      B   C
ATOM  3160 CG1 ILE B 149     11.099  83.891  33.071  1.00 14.05      B   C
ATOM  3161 CD1 ILE B 149      9.694  84.067  33.608  1.00 15.21      B   C
ATOM  3162 C   ILE B 149     14.742  83.842  34.386  1.00 12.66      B   C
ATOM  3163 O   ILE B 149     15.403  84.852  34.172  1.00 11.51      B   O
ATOM  3164 N   GLU B 150     15.041  82.995  35.366  1.00 12.92      B   N
ATOM  3165 CA  GLU B 150     16.180  83.266  36.235  1.00 13.66      B   C
ATOM  3166 CB  GLU B 150     16.182  82.313  37.441  1.00 18.92      B   C
ATOM  3167 CG  GLU B 150     14.884  82.371  38.242  1.00 23.46      B   C
ATOM  3168 CD  GLU B 150     15.024  81.875  39.673  1.00 28.25      B   C
ATOM  3169 OE1 GLU B 150     15.728  80.863  39.887  1.00 30.76      B   O
ATOM  3170 OE2 GLU B 150     14.414  82.491  40.581  1.00 24.21      B   O
ATOM  3171 C   GLU B 150     17.491  83.163  35.462  1.00 13.99      B   C
ATOM  3172 O   GLU B 150     18.484  83.776  35.844  1.00 14.58      B   O
ATOM  3173 N   GLU B 151     17.500  82.403  34.370  1.00 13.36      B   N
ATOM  3174 CA  GLU B 151     18.712  82.277  33.571  1.00 16.12      B   C
ATOM  3175 CB  GLU B 151     18.863  80.861  33.006  1.00 18.99      B   C
ATOM  3176 CG  GLU B 151     20.276  80.598  32.500  1.00 25.66      B   C
ATOM  3177 CD  GLU B 151     20.615  79.128  32.403  1.00 27.80      B   C
ATOM  3178 OE1 GLU B 151     20.307  78.389  33.362  1.00 33.36      B   O
ATOM  3179 OE2 GLU B 151     21.204  78.716  31.378  1.00 24.62      B   O
ATOM  3180 C   GLU B 151     18.695  83.293  32.436  1.00 15.49      B   C
ATOM  3181 O   GLU B 151     19.515  83.243  31.522  1.00 16.76      B   O
ATOM  3182 N   SER B 152     17.746  84.218  32.514  1.00 15.83      B   N
ATOM  3183 CA  SER B 152     17.591  85.277  31.523  1.00 16.90      B   C
ATOM  3184 CB  SER B 152     18.843  86.159  31.486  1.00 16.89      B   C
ATOM  3185 OG  SER B 152     18.547  87.404  30.872  1.00 19.93      B   O
ATOM  3186 C   SER B 152     17.274  84.786  30.108  1.00 15.72      B   C
ATOM  3187 O   SER B 152     17.776  85.339  29.128  1.00 16.57      B   O
ATOM  3188 N   ILE B 153     16.452  83.746  30.003  1.00 16.59      B   N
ATOM  3189 CA  ILE B 153     16.048  83.223  28.701  1.00 16.23      B   C
ATOM  3190 CB  ILE B 153     15.840  81.688  28.747  1.00 17.80      B   C
ATOM  3191 CG2 ILE B 153     15.479  81.164  27.366  1.00 16.97      B   C
ATOM  3192 CG1 ILE B 153     17.118  81.008  29.247  1.00 18.17      B   C
ATOM  3193 CD1 ILE B 153     18.328  81.264  28.379  1.00 20.45      B   C
ATOM  3194 C   ILE B 153     14.716  83.924  28.465  1.00 17.00      B   C
ATOM  3195 O   ILE B 153     13.647  83.337  28.649  1.00 16.86      B   O
ATOM  3196 N   LEU B 154     14.802  85.192  28.074  1.00 16.13      B   N
ATOM  3197 CA  LEU B 154     13.629  86.036  27.861  1.00 17.93      B   C
ATOM  3198 CB  LEU B 154     13.891  87.412  28.475  1.00 15.30      B   C
ATOM  3199 CG  LEU B 154     14.390  87.335  29.923  1.00 14.99      B   C
ATOM  3200 CD1 LEU B 154     14.685  88.728  30.459  1.00 17.09      B   C
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Figure 6EEE

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ATOM  3201 CD2 LEU B 154    13.348  86.640  30.776  1.00 18.19    B   C
ATOM  3202 C   LEU B 154    13.188  86.204  26.413  1.00 19.02    B   C
ATOM  3203 O   LEU B 154    12.258  86.956  26.125  1.00 18.98    B   O
ATOM  3204 N   GLU B 155    13.857  85.506  25.506  1.00 19.46    B   N
ATOM  3205 CA  GLU B 155    13.520  85.579  24.093  1.00 20.61    B   C
ATOM  3206 CB  GLU B 155    14.055  86.877  23.481  1.00 23.20    B   C
ATOM  3207 CG  GLU B 155    15.563  86.894  23.285  1.00 31.50    B   C
ATOM  3208 CD  GLU B 155    16.077  88.235  22.778  1.00 39.23    B   C
ATOM  3209 OE1 GLU B 155    15.483  88.786  21.824  1.00 42.91    B   O
ATOM  3210 OE2 GLU B 155    17.084  88.734  23.328  1.00 43.36    B   O
ATOM  3211 C   GLU B 155    14.177  84.391  23.421  1.00 19.99    B   C
ATOM  3212 O   GLU B 155    14.864  83.610  24.077  1.00 21.64    B   O
ATOM  3213 N   GLY B 156    13.946  84.242  22.121  1.00 20.12    B   N
ATOM  3214 CA  GLY B 156    14.563  83.152  21.396  1.00 19.17    B   C
ATOM  3215 C   GLY B 156    13.844  81.820  21.366  1.00 20.79    B   C
ATOM  3216 O   GLY B 156    12.804  81.618  21.995  1.00 18.13    B   O
ATOM  3217 N   GLU B 157    14.451  80.898  20.626  1.00 22.19    B   N
ATOM  3218 CA  GLU B 157    13.946  79.548  20.415  1.00 21.56    B   C
ATOM  3219 CB  GLU B 157    14.952  78.782  19.553  1.00 25.02    B   C
ATOM  3220 CG  GLU B 157    14.524  77.377  19.184  1.00 35.87    B   C
ATOM  3221 CD  GLU B 157    15.499  76.703  18.231  1.00 41.09    B   C
ATOM  3222 OE1 GLU B 157    16.701  76.596  18.573  1.00 42.82    B   O
ATOM  3223 OE2 GLU B 157    15.058  76.275  17.141  1.00 42.70    B   O
ATOM  3224 C   GLU B 157    13.613  78.732  21.666  1.00 20.08    B   C
ATOM  3225 O   GLU B 157    12.588  78.044  21.702  1.00 18.27    B   O
ATOM  3226 N   LEU B 158    14.471  78.796  22.683  1.00 17.09    B   N
ATOM  3227 CA  LEU B 158    14.238  78.033  23.904  1.00 15.87    B   C
ATOM  3228 CB  LEU B 158    15.447  78.132  24.842  1.00 18.05    B   C
ATOM  3229 CG  LEU B 158    15.334  77.315  26.136  1.00 17.16    B   C
ATOM  3230 CD1 LEU B 158    14.977  75.872  25.807  1.00 15.66    B   C
ATOM  3231 CD2 LEU B 158    16.651  77.382  26.905  1.00 17.03    B   C
ATOM  3232 C   LEU B 158    12.973  78.488  24.630  1.00 16.52    B   C
ATOM  3233 O   LEU B 158    12.189  77.662  25.108  1.00 14.49    B   O
ATOM  3234 N   LEU B 159    12.775  79.799  24.727  1.00 14.92    B   N
ATOM  3235 CA  LEU B 159    11.580  80.306  25.383  1.00 14.51    B   C
ATOM  3236 CB  LEU B 159    11.660  81.823  25.578  1.00 15.13    B   C
ATOM  3237 CG  LEU B 159    10.374  82.456  26.133  1.00 16.38    B   C
ATOM  3238 CD1 LEU B 159     9.996  81.799  27.450  1.00 14.88    B   C
ATOM  3239 CD2 LEU B 159    10.574  83.955  26.326  1.00 15.09    B   C
ATOM  3240 C   LEU B 159    10.367  79.951  24.519  1.00 14.59    B   C
ATOM  3241 O   LEU B 159     9.350  79.492  25.028  1.00 13.56    B   O
ATOM  3242 N   GLU B 160    10.483  80.150  23.209  1.00 14.14    B   N
ATOM  3243 CA  GLU B 160     9.382  79.820  22.304  1.00 16.06    B   C
ATOM  3244 CB  GLU B 160     9.779  80.107  20.853  1.00 18.15    B   C
ATOM  3245 CG  GLU B 160     8.709  79.743  19.815  1.00 23.84    B   C
ATOM  3246 CD  GLU B 160     7.357  80.384  20.107  1.00 27.35    B   C
ATOM  3247 OE1 GLU B 160     7.330  81.496  20.683  1.00 24.13    B   O
ATOM  3248 OE2 GLU B 160     6.321  79.783  19.748  1.00 30.37    B   O
ATOM  3249 C   GLU B 160     8.987  78.348  22.438  1.00 15.10    B   C
ATOM  3250 O   GLU B 160     7.811  78.015  22.566  1.00 16.67    B   O
ATOM  3251 N   THR B 161     9.979  77.469  22.416  1.00 15.36    B   N
ATOM  3252 CA  THR B 161     9.720  76.037  22.518  1.00 16.10    B   C
ATOM  3253 CB  THR B 161    11.024  75.243  22.343  1.00 17.81    B   C
ATOM  3254 OG1 THR B 161    11.607  75.567  21.072  1.00 19.62    B   O
ATOM  3255 CG2 THR B 161    10.756  73.748  22.407  1.00 18.12    B   C
ATOM  3256 C   THR B 161     9.066  75.676  23.851  1.00 14.89    B   C
ATOM  3257 O   THR B 161     8.172  74.821  23.907  1.00 13.07    B   O
ATOM  3258 N   CYS B 162     9.500  76.342  24.918  1.00 12.65    B   N
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Figure 6FFF

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ATOM  3259 CA  CYS B 162     8.958  76.087  26.248  1.00 15.38    B   C
ATOM  3260 CB  CYS B 162     9.800  76.796  27.310  1.00 14.79    B   C
ATOM  3261 SG  CYS B 162     9.400  76.328  29.021  1.00 16.89    B   S
ATOM  3262 C   CYS B 162     7.505  76.557  26.341  1.00 15.60    B   C
ATOM  3263 O   CYS B 162     6.651  75.849  26.877  1.00 15.21    B   O
ATOM  3264 N   MET B 163     7.226  77.756  25.831  1.00 15.17    B   N
ATOM  3265 CA  MET B 163     5.863  78.271  25.860  1.00 15.78    B   C
ATOM  3266 CB  MET B 163     5.792  79.695  25.294  1.00 15.75    B   C
ATOM  3267 CG  MET B 163     6.424  80.767  26.162  1.00 16.77    B   C
ATOM  3268 SD  MET B 163     5.978  82.432  25.603  1.00 16.61    B   S
ATOM  3269 CE  MET B 163     6.937  82.509  24.114  1.00 14.38    B   C
ATOM  3270 C   MET B 163     4.962  77.360  25.033  1.00 14.99    B   C
ATOM  3271 O   MET B 163     3.819  77.093  25.410  1.00 15.77    B   O
ATOM  3272 N   HIS B 164     5.484  76.879  23.909  1.00 15.34    B   N
ATOM  3273 CA  HIS B 164     4.718  76.002  23.033  1.00 19.25    B   C
ATOM  3274 CB  HIS B 164     5.504  75.724  21.751  1.00 20.62    B   C
ATOM  3275 CG  HIS B 164     4.693  75.055  20.688  1.00 28.25    B   C
ATOM  3276 CD2 HIS B 164     4.779  73.817  20.146  1.00 28.01    B   C
ATOM  3277 ND1 HIS B 164     3.608  75.661  20.090  1.00 29.20    B   N
ATOM  3278 CE1 HIS B 164     3.060  74.824  19.227  1.00 29.23    B   C
ATOM  3279 NE2 HIS B 164     3.750  73.698  19.243  1.00 29.55    B   N
ATOM  3280 C   HIS B 164     4.412  74.690  23.760  1.00 19.47    B   C
ATOM  3281 O   HIS B 164     3.293  74.169  23.704  1.00 17.49    B   O
ATOM  3282 N   TYR B 165     5.419  74.169  24.449  1.00 17.68    B   N
ATOM  3283 CA  TYR B 165     5.277  72.937  25.210  1.00 16.69    B   C
ATOM  3284 CB  TYR B 165     6.578  72.655  25.969  1.00 15.68    B   C
ATOM  3285 CG  TYR B 165     6.457  71.544  26.976  1.00 17.57    B   C
ATOM  3286 CD1 TYR B 165     6.384  70.211  26.569  1.00 16.95    B   C
ATOM  3287 CE1 TYR B 165     6.216  69.191  27.498  1.00 20.45    B   C
ATOM  3288 CD2 TYR B 165     6.362  71.829  28.336  1.00 15.75    B   C
ATOM  3289 CE2 TYR B 165     6.193  70.818  29.273  1.00 17.81    B   C
ATOM  3290 CZ  TYR B 165     6.119  69.501  28.847  1.00 18.80    B   C
ATOM  3291 OH  TYR B 165     5.941  68.500  29.773  1.00 19.07    B   O
ATOM  3292 C   TYR B 165     4.101  73.027  26.193  1.00 16.83    B   C
ATOM  3293 O   TYR B 165     3.303  72.094  26.310  1.00 19.76    B   O
ATOM  3294 N   TYR B 166     3.999  74.151  26.895  1.00 16.40    B   N
ATOM  3295 CA  TYR B 166     2.931  74.369  27.864  1.00 16.70    B   C
ATOM  3296 CB  TYR B 166     3.362  75.435  28.888  1.00 13.68    B   C
ATOM  3297 CG  TYR B 166     4.354  74.961  29.930  1.00 15.63    B   C
ATOM  3298 CD1 TYR B 166     5.545  75.650  30.150  1.00 13.48    B   C
ATOM  3299 CE1 TYR B 166     6.458  75.218  31.113  1.00 17.41    B   C
ATOM  3300 CD2 TYR B 166     4.097  73.825  30.702  1.00 16.97    B   C
ATOM  3301 CE2 TYR B 166     5.001  73.387  31.668  1.00 14.41    B   C
ATOM  3302 CZ  TYR B 166     6.176  74.084  31.868  1.00 15.99    B   C
ATOM  3303 OH  TYR B 166     7.058  73.648  32.827  1.00 15.83    B   O
ATOM  3304 C   TYR B 166     1.576  74.793  27.278  1.00 17.53    B   C
ATOM  3305 O   TYR B 166     0.529  74.344  27.746  1.00 18.77    B   O
ATOM  3306 N   PHE B 167     1.599  75.651  26.260  1.00 18.80    B   N
ATOM  3307 CA  PHE B 167     0.367  76.198  25.668  1.00 19.74    B   C
ATOM  3308 CB  PHE B 167     0.660  77.589  25.115  1.00 18.42    B   C
ATOM  3309 CG  PHE B 167     1.092  78.573  26.163  1.00 17.20    B   C
ATOM  3310 CD1 PHE B 167     1.928  79.627  25.824  1.00 16.80    B   C
ATOM  3311 CD2 PHE B 167     0.635  78.472  27.482  1.00 16.87    B   C
ATOM  3312 CE1 PHE B 167     2.306  80.572  26.770  1.00 17.05    B   C
ATOM  3313 CE2 PHE B 167     1.010  79.419  28.439  1.00 17.71    B   C
ATOM  3314 CZ  PHE B 167     1.851  80.472  28.075  1.00 17.51    B   C
ATOM  3315 C   PHE B 167    -0.367  75.383  24.618  1.00 21.10    B   C
ATOM  3316 O   PHE B 167    -1.597  75.430  24.535  1.00 19.22    B   O
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Figure 6GGG

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ATOM  3317 N   THR B 168     0.403  74.657  23.812  1.00 23.27    B   N
ATOM  3318 CA  THR B 168    -0.165  73.805  22.765  1.00 26.77    B   C
ATOM  3319 CB  THR B 168     0.865  72.832  22.187  1.00 27.57    B   C
ATOM  3320 OG1 THR B 168     1.911  73.535  21.517  1.00 32.03    B   O
ATOM  3321 CG2 THR B 168     0.186  71.880  21.180  1.00 32.54    B   C
ATOM  3322 C   THR B 168    -1.363  72.944  23.205  1.00 26.77    B   C
ATOM  3323 O   THR B 168    -2.395  72.938  22.572  1.00 28.26    B   O
ATOM  3324 N   PRO B 169    -1.239  72.197  24.326  1.00 26.46    B   N
ATOM  3325 CD  PRO B 169    -0.050  72.083  25.152  1.00 26.67    B   C
ATOM  3326 CA  PRO B 169    -2.291  71.326  24.883  1.00 25.55    B   C
ATOM  3327 CB  PRO B 169    -1.610  70.668  26.066  1.00 26.50    B   C
ATOM  3328 CG  PRO B 169    -0.169  70.666  25.699  1.00 26.43    B   C
ATOM  3329 C   PRO B 169    -3.593  72.077  25.297  1.00 24.82    B   C
ATOM  3330 O   PRO B 169    -4.610  71.418  25.576  1.00 24.34    B   O
ATOM  3331 N   LEU B 170    -3.536  73.405  25.391  1.00 22.80    B   N
ATOM  3332 CA  LEU B 170    -4.729  74.167  25.761  1.00 25.50    B   C
ATOM  3333 CB  LEU B 170    -4.385  75.632  25.964  1.00 23.84    B   C
ATOM  3334 CG  LEU B 170    -3.514  75.982  27.186  1.00 25.53    B   C
ATOM  3335 CD1 LEU B 170    -3.138  77.463  27.146  1.00 26.01    B   C
ATOM  3336 CD2 LEU B 170    -4.242  75.652  28.503  1.00 26.09    B   C
ATOM  3337 C   LEU B 170    -5.772  74.057  24.644  1.00 25.77    B   C
ATOM  3338 O   LEU B 170    -5.436  74.103  23.453  1.00 26.97    B   O
ATOM  3339 N   GLU B 171    -7.033  73.952  25.037  1.00 27.92    B   N
ATOM  3340 CA  GLU B 171    -8.117  73.860  24.078  1.00 30.46    B   C
ATOM  3341 CB  GLU B 171    -9.035  72.693  24.435  1.00 34.23    B   C
ATOM  3342 CG  GLU B 171    -8.408  71.310  24.268  1.00 36.53    B   C
ATOM  3343 CD  GLU B 171    -7.963  71.029  22.844  1.00 38.06    B   C
ATOM  3344 OE1 GLU B 171    -8.773  71.218  21.911  1.00 38.60    B   O
ATOM  3345 OE2 GLU B 171    -6.800  70.614  22.659  1.00 38.27    B   O
ATOM  3346 C   GLU B 171    -8.903  75.155  24.104  1.00 30.56    B   C
ATOM  3347 O   GLU B 171    -9.477  75.560  23.093  1.00 33.13    B   O
ATOM  3348 N   ILE B 172    -8.922  75.801  25.265  1.00 27.64    B   N
ATOM  3349 CA  ILE B 172    -9.627  77.060  25.428  1.00 26.46    B   C
ATOM  3350 CB  ILE B 172   -10.239  77.179  26.838  1.00 26.68    B   C
ATOM  3351 CG2 ILE B 172   -10.916  78.534  26.994  1.00 26.23    B   C
ATOM  3352 CG1 ILE B 172   -11.246  76.050  27.071  1.00 27.08    B   C
ATOM  3353 CD1 ILE B 172   -11.899  76.085  28.443  1.00 27.76    B   C
ATOM  3354 C   ILE B 172    -8.670  78.225  25.218  1.00 26.74    B   C
ATOM  3355 O   ILE B 172    -7.604  78.284  25.833  1.00 24.89    B   O
ATOM  3356 N   LEU B 173    -9.055  79.148  24.343  1.00 25.65    B   N
ATOM  3357 CA  LEU B 173    -8.245  80.328  24.061  1.00 25.77    B   C
ATOM  3358 CB  LEU B 173    -8.564  80.853  22.659  1.00 28.20    B   C
ATOM  3359 CG  LEU B 173    -7.682  81.962  22.082  1.00 29.17    B   C
ATOM  3360 CD1 LEU B 173    -6.227  81.521  22.081  1.00 31.35    B   C
ATOM  3361 CD2 LEU B 173    -8.144  82.281  20.661  1.00 29.98    B   C
ATOM  3362 C   LEU B 173    -8.585  81.387  25.111  1.00 24.69    B   C
ATOM  3363 O   LEU B 173    -9.720  81.852  25.188  1.00 26.80    B   O
ATOM  3364 N   PRO B 174    -7.606  81.780  25.939  1.00 21.86    B   N
ATOM  3365 CD  PRO B 174    -6.227  81.269  26.032  1.00 20.12    B   C
ATOM  3366 CA  PRO B 174    -7.857  82.786  26.973  1.00 21.00    B   C
ATOM  3367 CB  PRO B 174    -6.629  82.663  27.873  1.00 20.86    B   C
ATOM  3368 CG  PRO B 174    -5.553  82.313  26.900  1.00 20.88    B   C
ATOM  3369 C   PRO B 174    -8.058  84.215  26.481  1.00 21.07    B   C
ATOM  3370 O   PRO B 174    -7.442  84.652  25.510  1.00 20.92    B   O
ATOM  3371 N   GLU B 175    -8.941  84.932  27.163  1.00 20.88    B   N
ATOM  3372 CA  GLU B 175    -9.210  86.325  26.849  1.00 20.49    B   C
ATOM  3373 CB  GLU B 175   -10.714  86.599  26.886  1.00 22.18    B   C
ATOM  3374 CG  GLU B 175   -11.414  86.262  25.584  1.00 24.72    B   C
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Figure 6HHH

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ATOM  3375 CD  GLU B 175    -12.914  86.445  25.662  1.00 27.87    B   C
ATOM  3376 OE1 GLU B 175    -13.362  87.355  26.386  1.00 29.73    B   O
ATOM  3377 OE2 GLU B 175    -13.643  85.686  24.989  1.00 30.38    B   O
ATOM  3378 C   GLU B 175     -8.492  87.110  27.932  1.00 19.76    B   C
ATOM  3379 O   GLU B 175     -8.151  88.278  27.760  1.00 19.06    B   O
ATOM  3380 N   VAL B 176     -8.249  86.429  29.047  1.00 18.72    B   N
ATOM  3381 CA  VAL B 176     -7.561  87.013  30.187  1.00 18.26    B   C
ATOM  3382 CB  VAL B 176     -8.542  87.366  31.329  1.00 19.04    B   C
ATOM  3383 CG1 VAL B 176     -7.792  88.005  32.473  1.00 17.96    B   C
ATOM  3384 CG2 VAL B 176     -9.627  88.307  30.819  1.00 19.77    B   C
ATOM  3385 C   VAL B 176     -6.566  85.994  30.728  1.00 18.77    B   C
ATOM  3386 O   VAL B 176     -6.909  84.830  30.936  1.00 18.44    B   O
ATOM  3387 N   ILE B 177     -5.337  86.438  30.955  1.00 15.78    B   N
ATOM  3388 CA  ILE B 177     -4.302  85.564  31.485  1.00 15.67    B   C
ATOM  3389 CB  ILE B 177     -3.149  85.366  30.479  1.00 16.57    B   C
ATOM  3390 CG2 ILE B 177     -2.076  84.471  31.092  1.00 15.73    B   C
ATOM  3391 CG1 ILE B 177     -3.679  84.754  29.184  1.00 17.67    B   C
ATOM  3392 CD1 ILE B 177     -2.639  84.634  28.094  1.00 16.12    B   C
ATOM  3393 C   ILE B 177     -3.730  86.191  32.746  1.00 15.83    B   C
ATOM  3394 O   ILE B 177     -3.319  87.356  32.742  1.00 15.47    B   O
ATOM  3395 N   ILE B 178     -3.721  85.427  33.832  1.00 15.84    B   N
ATOM  3396 CA  ILE B 178     -3.178  85.932  35.080  1.00 15.63    B   C
ATOM  3397 CB  ILE B 178     -3.958  85.402  36.314  1.00 16.93    B   C
ATOM  3398 CG2 ILE B 178     -3.370  85.986  37.589  1.00 15.87    B   C
ATOM  3399 CG1 ILE B 178     -5.432  85.807  36.228  1.00 18.02    B   C
ATOM  3400 CD1 ILE B 178     -6.267  85.341  37.422  1.00 17.46    B   C
ATOM  3401 C   ILE B 178     -1.724  85.486  35.190  1.00 14.02    B   C
ATOM  3402 O   ILE B 178     -1.416  84.300  35.089  1.00 13.65    B   O
ATOM  3403 N   LEU B 179     -0.833  86.449  35.376  1.00 14.12    B   N
ATOM  3404 CA  LEU B 179      0.589  86.150  35.525  1.00 14.34    B   C
ATOM  3405 CB  LEU B 179      1.428  87.340  35.053  1.00 15.34    B   C
ATOM  3406 CG  LEU B 179      1.169  87.783  33.610  1.00 16.04    B   C
ATOM  3407 CD1 LEU B 179      1.942  89.073  33.332  1.00 18.24    B   C
ATOM  3408 CD2 LEU B 179      1.574  86.680  32.636  1.00 16.26    B   C
ATOM  3409 C   LEU B 179      0.783  85.915  37.021  1.00 14.01    B   C
ATOM  3410 O   LEU B 179      1.391  86.727  37.719  1.00 13.42    B   O
ATOM  3411 N   GLY B 180      0.252  84.790  37.493  1.00 13.50    B   N
ATOM  3412 CA  GLY B 180      0.310  84.448  38.906  1.00 13.79    B   C
ATOM  3413 C   GLY B 180      1.632  83.927  39.417  1.00 12.30    B   C
ATOM  3414 O   GLY B 180      1.681  82.902  40.093  1.00 14.02    B   O
ATOM  3415 N   CYS B 181      2.702  84.647  39.093  1.00 13.12    B   N
ATOM  3416 CA  CYS B 181      4.048  84.295  39.518  1.00 11.26    B   C
ATOM  3417 CB  CYS B 181      4.591  83.150  38.667  1.00 11.52    B   C
ATOM  3418 SG  CYS B 181      6.279  82.671  39.091  1.00 14.29    B   S
ATOM  3419 C   CYS B 181      4.927  85.532  39.348  1.00 11.67    B   C
ATOM  3420 O   CYS B 181      4.837  86.226  38.336  1.00 10.15    B   O
ATOM  3421 N   THR B 182      5.770  85.796  40.342  1.00 10.95    B   N
ATOM  3422 CA  THR B 182      6.671  86.950  40.329  1.00 11.68    B   C
ATOM  3423 CB  THR B 182      7.654  86.902  41.517  1.00 12.29    B   C
ATOM  3424 OG1 THR B 182      8.306  85.623  41.546  1.00  8.82    B   O
ATOM  3425 CG2 THR B 182      6.918  87.133  42.832  1.00 13.05    B   C
ATOM  3426 C   THR B 182      7.511  87.085  39.068  1.00 12.00    B   C
ATOM  3427 O   THR B 182      7.775  88.190  38.604  1.00 11.14    B   O
ATOM  3428 N   HIS B 183      7.927  85.953  38.516  1.00 11.51    B   N
ATOM  3429 CA  HIS B 183      8.782  85.934  37.333  1.00 12.53    B   C
ATOM  3430 CB  HIS B 183      9.490  84.577  37.250  1.00 12.11    B   C
ATOM  3431 CG  HIS B 183     10.413  84.301  38.396  1.00 12.62    B   C
ATOM  3432 CD2 HIS B 183     11.662  83.774  38.425  1.00 14.37    B   C
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Figure 6III

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ATOM  3433 ND1 HIS B 183    10.074  84.558  39.708  1.00 12.87    B   N
ATOM  3434 CE1 HIS B 183    11.076  84.206  40.495  1.00 11.92    B   C
ATOM  3435 NE2 HIS B 183    12.051  83.728  39.741  1.00 12.64    B   N
ATOM  3436 C   HIS B 183    8.113  86.202  35.990  1.00 13.70    B   C
ATOM  3437 O   HIS B 183    8.735  86.757  35.082  1.00 14.63    B   O
ATOM  3438 N   PHE B 184    6.846  85.822  35.866  1.00 14.67    B   N
ATOM  3439 CA  PHE B 184    6.134  85.945  34.595  1.00 13.80    B   C
ATOM  3440 CB  PHE B 184    4.751  85.298  34.731  1.00 14.23    B   C
ATOM  3441 CG  PHE B 184    4.809  83.829  35.102  1.00 13.65    B   C
ATOM  3442 CD1 PHE B 184    3.646  83.084  35.240  1.00 16.74    B   C
ATOM  3443 CD2 PHE B 184    6.035  83.207  35.355  1.00 14.92    B   C
ATOM  3444 CE1 PHE B 184    3.698  81.743  35.631  1.00 13.35    B   C
ATOM  3445 CE2 PHE B 184    6.097  81.866  35.746  1.00 14.40    B   C
ATOM  3446 CZ  PHE B 184    4.923  81.136  35.884  1.00 13.35    B   C
ATOM  3447 C   PHE B 184    6.049  87.314  33.921  1.00 13.82    B   C
ATOM  3448 O   PHE B 184    5.991  87.391  32.691  1.00 13.30    B   O
ATOM  3449 N   PRO B 185    6.032  88.409  34.697  1.00 13.55    B   N
ATOM  3450 CD  PRO B 185    5.786  88.577  36.143  1.00 14.61    B   C
ATOM  3451 CA  PRO B 185    5.966  89.701  34.008  1.00 14.00    B   C
ATOM  3452 CB  PRO B 185    5.964  90.702  35.158  1.00 15.55    B   C
ATOM  3453 CG  PRO B 185    5.186  89.971  36.210  1.00 16.68    B   C
ATOM  3454 C   PRO B 185    7.158  89.907  33.063  1.00 14.41    B   C
ATOM  3455 O   PRO B 185    7.057  90.640  32.076  1.00 14.66    B   O
ATOM  3456 N   LEU B 186    8.285  89.257  33.355  1.00 13.60    B   N
ATOM  3457 CA  LEU B 186    9.462  89.410  32.503  1.00 14.78    B   C
ATOM  3458 CB  LEU B 186    10.707  88.844  33.185  1.00 16.45    B   C
ATOM  3459 CG  LEU B 186    11.268  89.716  34.312  1.00 17.76    B   C
ATOM  3460 CD1 LEU B 186    12.601  89.149  34.788  1.00 18.57    B   C
ATOM  3461 CD2 LEU B 186    11.454  91.145  33.800  1.00 19.96    B   C
ATOM  3462 C   LEU B 186    9.299  88.796  31.115  1.00 14.26    B   C
ATOM  3463 O   LEU B 186    10.105  89.060  30.219  1.00 13.67    B   O
ATOM  3464 N   ILE B 187    8.271  87.973  30.933  1.00 13.72    B   N
ATOM  3465 CA  ILE B 187    8.007  87.391  29.616  1.00 14.52    B   C
ATOM  3466 CB  ILE B 187    8.252  85.852  29.567  1.00 16.13    B   C
ATOM  3467 CG2 ILE B 187    9.734  85.563  29.730  1.00 15.11    B   C
ATOM  3468 CG1 ILE B 187    7.418  85.134  30.630  1.00 14.95    B   C
ATOM  3469 CD1 ILE B 187    7.386  83.616  30.452  1.00 18.91    B   C
ATOM  3470 C   ILE B 187    6.559  87.681  29.216  1.00 15.97    B   C
ATOM  3471 O   ILE B 187    5.970  86.973  28.399  1.00 14.41    B   O
ATOM  3472 N   ALA B 188    6.003  88.742  29.790  1.00 14.30    B   N
ATOM  3473 CA  ALA B 188    4.623  89.138  29.511  1.00 16.72    B   C
ATOM  3474 CB  ALA B 188    4.261  90.381  30.318  1.00 17.73    B   C
ATOM  3475 C   ALA B 188    4.386  89.386  28.021  1.00 17.75    B   C
ATOM  3476 O   ALA B 188    3.473  88.806  27.437  1.00 15.55    B   O
ATOM  3477 N   GLN B 189    5.208  90.232  27.404  1.00 18.64    B   N
ATOM  3478 CA  GLN B 189    5.045  90.521  25.979  1.00 20.60    B   C
ATOM  3479 CB  GLN B 189    5.977  91.668  25.553  1.00 24.25    B   C
ATOM  3480 CG  GLN B 189    7.448  91.297  25.369  1.00 34.75    B   C
ATOM  3481 CD  GLN B 189    8.385  92.508  25.450  1.00 39.99    B   C
ATOM  3482 OE1 GLN B 189    7.963  93.653  25.263  1.00 43.74    B   O
ATOM  3483 NE2 GLN B 189    9.663  92.254  25.720  1.00 40.19    B   N
ATOM  3484 C   GLN B 189    5.279  89.273  25.111  1.00 17.97    B   C
ATOM  3485 O   GLN B 189    4.729  89.163  24.015  1.00 14.32    B   O
ATOM  3486 N   LYS B 190    6.078  88.329  25.606  1.00 17.40    B   N
ATOM  3487 CA  LYS B 190    6.341  87.097  24.859  1.00 16.80    B   C
ATOM  3488 CB  LYS B 190    7.567  86.374  25.421  1.00 18.22    B   C
ATOM  3489 CG  LYS B 190    8.878  87.117  25.218  1.00 21.88    B   C
ATOM  3490 CD  LYS B 190    9.211  87.269  23.740  1.00 25.45    B   C
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Figure 6JJJ

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ATOM  3491  CE  LYS B 190      10.416  88.179  23.543  1.00 29.36      B   C
ATOM  3492  NZ  LYS B 190      10.790  88.298  22.110  1.00 29.28      B   N
ATOM  3493  C   LYS B 190       5.123  86.176  24.920  1.00 16.76      B   C
ATOM  3494  O   LYS B 190       4.775  85.521  23.934  1.00 15.72      B   O
ATOM  3495  N   ILE B 191       4.484  86.118  26.085  1.00 17.36      B   N
ATOM  3496  CA  ILE B 191       3.293  85.293  26.250  1.00 16.65      B   C
ATOM  3497  CB  ILE B 191       2.835  85.283  27.722  1.00 16.29      B   C
ATOM  3498  CG2 ILE B 191       1.429  84.706  27.837  1.00 15.90      B   C
ATOM  3499  CG1 ILE B 191       3.827  84.472  28.561  1.00 14.41      B   C
ATOM  3500  CD1 ILE B 191       3.575  84.556  30.065  1.00 15.15      B   C
ATOM  3501  C   ILE B 191       2.206  85.902  25.371  1.00 17.73      B   C
ATOM  3502  O   ILE B 191       1.431  85.201  24.730  1.00 17.39      B   O
ATOM  3503  N   GLU B 192       2.174  87.227  25.343  1.00 19.90      B   N
ATOM  3504  CA  GLU B 192       1.206  87.955  24.545  1.00 20.35      B   C
ATOM  3505  CB  GLU B 192       1.368  89.452  24.811  1.00 22.52      B   C
ATOM  3506  CG  GLU B 192       0.186  90.301  24.426  1.00 31.49      B   C
ATOM  3507  CD  GLU B 192       0.310  91.705  24.981  1.00 36.51      B   C
ATOM  3508  OE1 GLU B 192       0.342  91.845  26.223  1.00 39.33      B   O
ATOM  3509  OE2 GLU B 192       0.384  92.660  24.179  1.00 38.77      B   O
ATOM  3510  C   GLU B 192       1.468  87.638  23.077  1.00 18.85      B   C
ATOM  3511  O   GLU B 192       0.553  87.274  22.327  1.00 18.00      B   O
ATOM  3512  N   GLY B 193       2.733  87.764  22.685  1.00 19.26      B   N
ATOM  3513  CA  GLY B 193       3.134  87.497  21.319  1.00 16.37      B   C
ATOM  3514  C   GLY B 193       2.843  86.078  20.880  1.00 17.40      B   C
ATOM  3515  O   GLY B 193       2.580  85.832  19.700  1.00 19.53      B   O
ATOM  3516  N   TYR B 194       2.892  85.138  21.819  1.00 15.60      B   N
ATOM  3517  CA  TYR B 194       2.621  83.740  21.494  1.00 16.39      B   C
ATOM  3518  CB  TYR B 194       2.829  82.845  22.715  1.00 16.47      B   C
ATOM  3519  CG  TYR B 194       2.502  81.386  22.452  1.00 15.75      B   C
ATOM  3520  CD1 TYR B 194       3.470  80.515  21.964  1.00 17.79      B   C
ATOM  3521  CE1 TYR B 194       3.171  79.178  21.698  1.00 18.26      B   C
ATOM  3522  CD2 TYR B 194       1.216  80.887  22.669  1.00 15.15      B   C
ATOM  3523  CE2 TYR B 194       0.904  79.551  22.403  1.00 16.44      B   C
ATOM  3524  CZ  TYR B 194       1.890  78.703  21.920  1.00 15.60      B   C
ATOM  3525  OH  TYR B 194       1.614  77.379  21.671  1.00 17.72      B   O
ATOM  3526  C   TYR B 194       1.189  83.551  21.003  1.00 16.01      B   C
ATOM  3527  O   TYR B 194       0.966  82.985  19.940  1.00 17.33      B   O
ATOM  3528  N   PHE B 195       0.218  84.011  21.785  1.00 17.37      B   N
ATOM  3529  CA  PHE B 195      -1.177  83.851  21.390  1.00 19.84      B   C
ATOM  3530  CB  PHE B 195      -2.108  84.174  22.563  1.00 20.48      B   C
ATOM  3531  CG  PHE B 195      -2.057  83.146  23.659  1.00 21.18      B   C
ATOM  3532  CD1 PHE B 195      -1.166  83.281  24.720  1.00 20.24      B   C
ATOM  3533  CD2 PHE B 195      -2.847  82.002  23.590  1.00 20.40      B   C
ATOM  3534  CE1 PHE B 195      -1.061  82.289  25.692  1.00 18.52      B   C
ATOM  3535  CE2 PHE B 195      -2.748  81.004  24.558  1.00 21.83      B   C
ATOM  3536  CZ  PHE B 195      -1.853  81.149  25.609  1.00 18.80      B   C
ATOM  3537  C   PHE B 195      -1.549  84.675  20.168  1.00 21.22      B   C
ATOM  3538  O   PHE B 195      -2.381  84.260  19.364  1.00 23.42      B   O
ATOM  3539  N   MET B 196      -0.920  85.835  20.018  1.00 20.91      B   N
ATOM  3540  CA  MET B 196      -1.191  86.691  18.874  1.00 22.63      B   C
ATOM  3541  CB  MET B 196      -0.632  88.096  19.110  1.00 21.19      B   C
ATOM  3542  CG  MET B 196      -1.454  88.939  20.066  1.00 21.47      B   C
ATOM  3543  SD  MET B 196      -3.106  89.333  19.420  1.00 22.89      B   S
ATOM  3544  CE  MET B 196      -2.734  90.738  18.369  1.00 25.90      B   C
ATOM  3545  C   MET B 196      -0.574  86.098  17.616  1.00 22.76      B   C
ATOM  3546  O   MET B 196      -1.034  86.365  16.510  1.00 22.32      B   O
ATOM  3547  N   GLY B 197       0.462  85.284  17.788  1.00 23.35      B   N
ATOM  3548  CA  GLY B 197       1.117  84.682  16.644  1.00 23.78      B   C
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Figure 6KKK

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ATOM  3549  C   GLY B 197      0.612  83.294  16.308  1.00 26.07    B   C
ATOM  3550  O   GLY B 197      0.757  82.836  15.178  1.00 27.06    B   O
ATOM  3551  N   HIS B 198      0.011  82.618  17.280  1.00 24.62    B   N
ATOM  3552  CA  HIS B 198     -0.489  81.270  17.052  1.00 25.26    B   C
ATOM  3553  CB  HIS B 198     -0.143  80.393  18.250  1.00 24.79    B   C
ATOM  3554  CG  HIS B 198      1.318  80.087  18.358  1.00 27.65    B   C
ATOM  3555  CD2 HIS B 198      2.369  80.867  18.706  1.00 27.06    B   C
ATOM  3556  ND1 HIS B 198      1.847  78.858  18.026  1.00 29.54    B   N
ATOM  3557  CE1 HIS B 198      3.161  78.896  18.162  1.00 28.74    B   C
ATOM  3558  NE2 HIS B 198      3.503  80.104  18.572  1.00 27.31    B   N
ATOM  3559  C   HIS B 198     -1.982  81.189  16.742  1.00 25.16    B   C
ATOM  3560  O   HIS B 198     -2.470  80.160  16.274  1.00 25.84    B   O
ATOM  3561  N   PHE B 199     -2.701  82.274  17.002  1.00 23.99    B   N
ATOM  3562  CA  PHE B 199     -4.134  82.323  16.731  1.00 25.24    B   C
ATOM  3563  CB  PHE B 199     -4.939  82.150  18.021  1.00 25.35    B   C
ATOM  3564  CG  PHE B 199     -4.641  80.875  18.754  1.00 25.83    B   C
ATOM  3565  CD1 PHE B 199     -3.499  80.763  19.543  1.00 25.81    B   C
ATOM  3566  CD2 PHE B 199     -5.486  79.776  18.634  1.00 26.63    B   C
ATOM  3567  CE1 PHE B 199     -3.202  79.571  20.204  1.00 25.90    B   C
ATOM  3568  CE2 PHE B 199     -5.200  78.574  19.292  1.00 27.07    B   C
ATOM  3569  CZ  PHE B 199     -4.053  78.476  20.078  1.00 25.59    B   C
ATOM  3570  C   PHE B 199     -4.488  83.658  16.085  1.00 25.45    B   C
ATOM  3571  O   PHE B 199     -3.741  84.633  16.202  1.00 26.05    B   O
ATOM  3572  N   ALA B 200     -5.624  83.698  15.397  1.00 25.36    B   N
ATOM  3573  CA  ALA B 200     -6.066  84.926  14.744  1.00 26.49    B   C
ATOM  3574  CB  ALA B 200     -6.945  84.592  13.543  1.00 27.04    B   C
ATOM  3575  C   ALA B 200     -6.842  85.770  15.748  1.00 25.75    B   C
ATOM  3576  O   ALA B 200     -8.035  85.555  15.951  1.00 27.07    B   O
ATOM  3577  N   LEU B 201     -6.162  86.723  16.380  1.00 26.03    B   N
ATOM  3578  CA  LEU B 201     -6.801  87.588  17.371  1.00 25.45    B   C
ATOM  3579  CB  LEU B 201     -6.206  87.345  18.762  1.00 26.37    B   C
ATOM  3580  CG  LEU B 201     -6.409  85.971  19.404  1.00 27.87    B   C
ATOM  3581  CD1 LEU B 201     -5.727  85.944  20.768  1.00 27.55    B   C
ATOM  3582  CD2 LEU B 201     -7.895  85.681  19.539  1.00 28.11    B   C
ATOM  3583  C   LEU B 201     -6.668  89.069  17.041  1.00 24.86    B   C
ATOM  3584  O   LEU B 201     -5.571  89.565  16.801  1.00 25.77    B   O
ATOM  3585  N   PRO B 202     -7.792  89.795  17.036  1.00 25.07    B   N
ATOM  3586  CD  PRO B 202     -9.159  89.302  17.284  1.00 27.27    B   C
ATOM  3587  CA  PRO B 202     -7.801  91.229  16.739  1.00 27.30    B   C
ATOM  3588  CB  PRO B 202     -9.286  91.530  16.571  1.00 26.61    B   C
ATOM  3589  CG  PRO B 202     -9.919  90.581  17.541  1.00 28.74    B   C
ATOM  3590  C   PRO B 202     -7.162  92.024  17.878  1.00 28.85    B   C
ATOM  3591  O   PRO B 202     -6.625  93.111  17.676  1.00 31.54    B   O
ATOM  3592  N   THR B 203     -7.228  91.467  19.080  1.00 29.83    B   N
ATOM  3593  CA  THR B 203     -6.649  92.104  20.253  1.00 30.73    B   C
ATOM  3594  CB  THR B 203     -7.717  92.910  21.029  1.00 32.69    B   C
ATOM  3595  OG1 THR B 203     -7.113  93.535  22.168  1.00 38.76    B   O
ATOM  3596  CG2 THR B 203     -8.854  92.009  21.478  1.00 34.49    B   C
ATOM  3597  C   THR B 203     -6.057  91.009  21.142  1.00 30.11    B   C
ATOM  3598  O   THR B 203     -6.632  89.929  21.281  1.00 29.77    B   O
ATOM  3599  N   PRO B 204     -4.888  91.271  21.746  1.00 28.28    B   N
ATOM  3600  CD  PRO B 204     -4.105  92.519  21.714  1.00 29.99    B   C
ATOM  3601  CA  PRO B 204     -4.249  90.278  22.608  1.00 25.72    B   C
ATOM  3602  CB  PRO B 204     -2.871  90.878  22.851  1.00 27.64    B   C
ATOM  3603  CG  PRO B 204     -3.170  92.344  22.895  1.00 30.54    B   C
ATOM  3604  C   PRO B 204     -5.007  90.034  23.906  1.00 22.99    B   C
ATOM  3605  O   PRO B 204     -5.829  90.847  24.322  1.00 21.45    B   O
ATOM  3606  N   PRO B 205     -4.754  88.888  24.550  1.00 23.17    B   N
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Figure 6LLL

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ATOM  3607 CD  PRO B 205     -3.967  87.734  24.079  1.00 22.14    B   C
ATOM  3608 CA  PRO B 205     -5.435  88.579  25.812  1.00 21.71    B   C
ATOM  3609 CB  PRO B 205     -4.930  87.177  26.145  1.00 20.02    B   C
ATOM  3610 CG  PRO B 205     -4.640  86.587  24.791  1.00 24.28    B   C
ATOM  3611 C   PRO B 205     -5.013  89.592  26.870  1.00 20.42    B   C
ATOM  3612 O   PRO B 205     -3.884  90.081  26.855  1.00 20.68    B   O
ATOM  3613 N   LEU B 206     -5.920  89.912  27.781  1.00 19.56    B   N
ATOM  3614 CA  LEU B 206     -5.614  90.852  28.844  1.00 18.19    B   C
ATOM  3615 CB  LEU B 206     -6.903  91.341  29.506  1.00 19.98    B   C
ATOM  3616 CG  LEU B 206     -6.733  92.187  30.772  1.00 20.16    B   C
ATOM  3617 CD1 LEU B 206     -6.025  93.490  30.435  1.00 20.32    B   C
ATOM  3618 CD2 LEU B 206     -8.097  92.461  31.383  1.00 21.77    B   C
ATOM  3619 C   LEU B 206     -4.748  90.152  29.887  1.00 19.09    B   C
ATOM  3620 O   LEU B 206     -5.155  89.137  30.460  1.00 16.01    B   O
ATOM  3621 N   LEU B 207     -3.554  90.682  30.130  1.00 17.87    B   N
ATOM  3622 CA  LEU B 207     -2.673  90.086  31.128  1.00 19.96    B   C
ATOM  3623 CB  LEU B 207     -1.204  90.137  30.683  1.00 20.75    B   C
ATOM  3624 CG  LEU B 207     -0.775  89.375  29.427  1.00 23.64    B   C
ATOM  3625 CD1 LEU B 207      0.754  89.247  29.409  1.00 24.69    B   C
ATOM  3626 CD2 LEU B 207     -1.402  88.003  29.411  1.00 25.49    B   C
ATOM  3627 C   LEU B 207     -2.822  90.826  32.450  1.00 18.55    B   C
ATOM  3628 O   LEU B 207     -2.846  92.056  32.489  1.00 19.17    B   O
ATOM  3629 N   ILE B 208     -2.925  90.067  33.534  1.00 17.96    B   N
ATOM  3630 CA  ILE B 208     -3.064  90.645  34.860  1.00 17.50    B   C
ATOM  3631 CB  ILE B 208     -4.118  89.878  35.685  1.00 17.43    B   C
ATOM  3632 CG2 ILE B 208     -4.243  90.491  37.077  1.00 18.18    B   C
ATOM  3633 CG1 ILE B 208     -5.459  89.892  34.943  1.00 18.45    B   C
ATOM  3634 CD1 ILE B 208     -6.012  91.289  34.699  1.00 14.50    B   C
ATOM  3635 C   ILE B 208     -1.719  90.585  35.575  1.00 16.82    B   C
ATOM  3636 O   ILE B 208     -1.164  89.508  35.780  1.00 15.89    B   O
ATOM  3637 N   HIS B 209     -1.213  91.756  35.950  1.00 17.14    B   N
ATOM  3638 CA  HIS B 209      0.074  91.899  36.632  1.00 18.16    B   C
ATOM  3639 CB  HIS B 209      0.745  93.175  36.106  1.00 18.91    B   C
ATOM  3640 CG  HIS B 209      2.193  93.306  36.457  1.00 20.99    B   C
ATOM  3641 CD2 HIS B 209      3.306  93.162  35.699  1.00 19.36    B   C
ATOM  3642 ND1 HIS B 209      2.629  93.657  37.716  1.00 22.36    B   N
ATOM  3643 CE1 HIS B 209      3.949  93.725  37.718  1.00 21.52    B   C
ATOM  3644 NE2 HIS B 209      4.384  93.429  36.506  1.00 15.94    B   N
ATOM  3645 C   HIS B 209     -0.149  91.980  38.150  1.00 17.31    B   C
ATOM  3646 O   HIS B 209     -0.909  92.826  38.621  1.00 17.80    B   O
ATOM  3647 N   SER B 210      0.513  91.104  38.908  1.00 15.90    B   N
ATOM  3648 CA  SER B 210      0.361  91.070  40.366  1.00 18.09    B   C
ATOM  3649 CB  SER B 210      1.187  89.931  40.975  1.00 15.92    B   C
ATOM  3650 OG  SER B 210      0.783  88.671  40.475  1.00 17.30    B   O
ATOM  3651 C   SER B 210      0.762  92.368  41.048  1.00 18.89    B   C
ATOM  3652 O   SER B 210      0.146  92.783  42.036  1.00 18.64    B   O
ATOM  3653 N   GLY B 211      1.806  92.999  40.527  1.00 18.49    B   N
ATOM  3654 CA  GLY B 211      2.276  94.241  41.105  1.00 17.93    B   C
ATOM  3655 C   GLY B 211      1.300  95.384  40.929  1.00 18.65    B   C
ATOM  3656 O   GLY B 211      0.988  96.088  41.888  1.00 18.89    B   O
ATOM  3657 N   ASP B 212      0.821  95.585  39.708  1.00 17.89    B   N
ATOM  3658 CA  ASP B 212     -0.122  96.666  39.454  1.00 19.78    B   C
ATOM  3659 CB  ASP B 212     -0.441  96.776  37.959  1.00 21.36    B   C
ATOM  3660 CG  ASP B 212      0.789  97.074  37.119  1.00 25.55    B   C
ATOM  3661 OD1 ASP B 212      1.588  97.954  37.509  1.00 24.93    B   O
ATOM  3662 OD2 ASP B 212      0.948  96.432  36.059  1.00 27.71    B   O
ATOM  3663 C   ASP B 212     -1.414  96.441  40.227  1.00 18.76    B   C
ATOM  3664 O   ASP B 212     -2.025  97.389  40.712  1.00 19.27    B   O
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Figure 6MMM

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ATOM  3665 N   ALA B 213    -1.825  95.182  40.344  1.00 19.86    B   N
ATOM  3666 CA  ALA B 213    -3.055  94.847  41.054  1.00 17.54    B   C
ATOM  3667 CB  ALA B 213    -3.378  93.372  40.876  1.00 17.05    B   C
ATOM  3668 C   ALA B 213    -2.959  95.183  42.539  1.00 19.06    B   C
ATOM  3669 O   ALA B 213    -3.901  95.725  43.120  1.00 16.90    B   O
ATOM  3670 N   ILE B 214    -1.823  94.876  43.158  1.00 15.97    B   N
ATOM  3671 CA  ILE B 214    -1.678  95.162  44.577  1.00 16.41    B   C
ATOM  3672 CB  ILE B 214    -0.503  94.357  45.206  1.00 17.51    B   C
ATOM  3673 CG2 ILE B 214     0.841  94.960  44.809  1.00 16.99    B   C
ATOM  3674 CG1 ILE B 214    -0.639  94.359  46.733  1.00 17.48    B   C
ATOM  3675 CD1 ILE B 214     0.283  93.366  47.436  1.00 20.67    B   C
ATOM  3676 C   ILE B 214    -1.516  96.656  44.864  1.00 16.49    B   C
ATOM  3677 O   ILE B 214    -1.933  97.133  45.917  1.00 16.10    B   O
ATOM  3678 N   VAL B 215    -0.927  97.403  43.933  1.00 16.36    B   N
ATOM  3679 CA  VAL B 215    -0.772  98.841  44.139  1.00 17.16    B   C
ATOM  3680 CB  VAL B 215    -0.016  99.509  42.964  1.00 19.48    B   C
ATOM  3681 CG1 VAL B 215    -0.179 101.017  43.027  1.00 17.77    B   C
ATOM  3682 CG2 VAL B 215     1.470  99.147  43.022  1.00 17.10    B   C
ATOM  3683 C   VAL B 215    -2.161  99.471  44.259  1.00 18.05    B   C
ATOM  3684 O   VAL B 215    -2.417 100.282  45.153  1.00 17.39    B   O
ATOM  3685 N   GLU B 216    -3.054  99.089  43.354  1.00 19.67    B   N
ATOM  3686 CA  GLU B 216    -4.411  99.617  43.357  1.00 21.54    B   C
ATOM  3687 CB  GLU B 216    -5.188  99.059  42.166  1.00 23.84    B   C
ATOM  3688 CG  GLU B 216    -4.815  99.727  40.853  1.00 26.87    B   C
ATOM  3689 CD  GLU B 216    -5.388  99.014  39.648  1.00 30.91    B   C
ATOM  3690 OE1 GLU B 216    -5.399  99.623  38.558  1.00 34.30    B   O
ATOM  3691 OE2 GLU B 216    -5.815  97.845  39.785  1.00 31.99    B   O
ATOM  3692 C   GLU B 216    -5.126  99.293  44.657  1.00 20.92    B   C
ATOM  3693 O   GLU B 216    -5.815 100.141  45.223  1.00 19.64    B   O
ATOM  3694 N   TYR B 217    -4.955  98.065  45.135  1.00 21.71    B   N
ATOM  3695 CA  TYR B 217    -5.583  97.649  46.386  1.00 21.99    B   C
ATOM  3696 CB  TYR B 217    -5.307  96.167  46.658  1.00 22.18    B   C
ATOM  3697 CG  TYR B 217    -5.831  95.693  47.995  1.00 20.53    B   C
ATOM  3698 CD1 TYR B 217    -7.199  95.534  48.213  1.00 22.61    B   C
ATOM  3699 CE1 TYR B 217    -7.692  95.113  49.456  1.00 20.09    B   C
ATOM  3700 CD2 TYR B 217    -4.961  95.422  49.051  1.00 19.57    B   C
ATOM  3701 CE2 TYR B 217    -5.440  95.002  50.293  1.00 19.82    B   C
ATOM  3702 CZ  TYR B 217    -6.807  94.849  50.488  1.00 20.38    B   C
ATOM  3703 OH  TYR B 217    -7.288  94.422  51.709  1.00 19.08    B   O
ATOM  3704 C   TYR B 217    -5.056  98.473  47.558  1.00 22.00    B   C
ATOM  3705 O   TYR B 217    -5.832  98.992  48.362  1.00 21.85    B   O
ATOM  3706 N   LEU B 218    -3.734  98.591  47.654  1.00 19.08    B   N
ATOM  3707 CA  LEU B 218    -3.113  99.341  48.740  1.00 19.40    B   C
ATOM  3708 CB  LEU B 218    -1.585  99.279  48.615  1.00 17.82    B   C
ATOM  3709 CG  LEU B 218    -0.941  97.888  48.742  1.00 18.28    B   C
ATOM  3710 CD1 LEU B 218     0.541  97.968  48.389  1.00 15.96    B   C
ATOM  3711 CD2 LEU B 218    -1.128  97.353  50.155  1.00 16.26    B   C
ATOM  3712 C   LEU B 218    -3.582 100.798  48.791  1.00 21.94    B   C
ATOM  3713 O   LEU B 218    -3.841 101.335  49.866  1.00 18.51    B   O
ATOM  3714 N   GLN B 219    -3.691 101.433  47.629  1.00 22.92    B   N
ATOM  3715 CA  GLN B 219    -4.139 102.822  47.562  1.00 24.80    B   C
ATOM  3716 CB  GLN B 219    -4.004 103.353  46.129  1.00 26.04    B   C
ATOM  3717 CG  GLN B 219    -2.577 103.325  45.592  1.00 28.25    B   C
ATOM  3718 CD  GLN B 219    -2.470 103.820  44.156  1.00 28.07    B   C
ATOM  3719 OE1 GLN B 219    -3.166 103.334  43.262  1.00 25.98    B   O
ATOM  3720 NE2 GLN B 219    -1.588 104.790  43.932  1.00 30.48    B   N
ATOM  3721 C   GLN B 219    -5.596 102.914  48.005  1.00 24.27    B   C
ATOM  3722 O   GLN B 219    -5.995 103.859  48.683  1.00 25.16    B   O
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Figure 6NNN

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ATOM  3723  N   GLN B 220     -6.375 101.912  47.620  1.00 24.30      B   N
ATOM  3724  CA  GLN B 220     -7.792 101.838  47.943  1.00 28.00      B   C
ATOM  3725  CB  GLN B 220     -8.410 100.663  47.184  1.00 31.02      B   C
ATOM  3726  CG  GLN B 220     -9.920 100.674  47.077  1.00 39.36      B   C
ATOM  3727  CD  GLN B 220    -10.411 101.639  46.020  1.00 44.14      B   C
ATOM  3728  OE1 GLN B 220    -10.260 102.854  46.154  1.00 47.44      B   O
ATOM  3729  NE2 GLN B 220    -10.995 101.101  44.954  1.00 47.51      B   N
ATOM  3730  C   GLN B 220     -8.013 101.635  49.444  1.00 29.46      B   C
ATOM  3731  O   GLN B 220     -8.553 102.499  50.137  1.00 28.33      B   O
ATOM  3732  N   LYS B 221     -7.570 100.477  49.927  1.00 29.84      B   N
ATOM  3733  CA  LYS B 221     -7.720 100.075  51.321  1.00 28.05      B   C
ATOM  3734  CB  LYS B 221     -7.249  98.626  51.477  1.00 29.20      B   C
ATOM  3735  CG  LYS B 221     -8.124  97.761  52.381  1.00 33.06      B   C
ATOM  3736  CD  LYS B 221     -8.114  98.242  53.817  1.00 34.46      B   C
ATOM  3737  CE  LYS B 221     -8.796  97.239  54.738  1.00 34.63      B   C
ATOM  3738  NZ  LYS B 221     -8.003  95.993  54.896  1.00 31.31      B   N
ATOM  3739  C   LYS B 221     -7.012 100.953  52.345  1.00 27.08      B   C
ATOM  3740  O   LYS B 221     -7.556 101.230  53.416  1.00 27.24      B   O
ATOM  3741  N   TYR B 222     -5.804 101.399  52.029  1.00 25.82      B   N
ATOM  3742  CA  TYR B 222     -5.052 102.212  52.973  1.00 27.04      B   C
ATOM  3743  CB  TYR B 222     -3.658 101.616  53.147  1.00 22.44      B   C
ATOM  3744  CG  TYR B 222     -3.708 100.166  53.576  1.00 22.86      B   C
ATOM  3745  CD1 TYR B 222     -4.156  99.815  54.854  1.00 19.32      B   C
ATOM  3746  CE1 TYR B 222     -4.258  98.484  55.243  1.00 19.44      B   C
ATOM  3747  CD2 TYR B 222     -3.357  99.134  52.694  1.00 20.72      B   C
ATOM  3748  CE2 TYR B 222     -3.456  97.792  53.078  1.00 19.21      B   C
ATOM  3749  CZ  TYR B 222     -3.909  97.482  54.351  1.00 19.82      B   C
ATOM  3750  OH  TYR B 222     -4.027  96.167  54.725  1.00 19.05      B   O
ATOM  3751  C   TYR B 222     -4.968 103.667  52.539  1.00 29.48      B   C
ATOM  3752  O   TYR B 222     -4.096 104.405  52.986  1.00 31.72      B   O
ATOM  3753  N   ALA B 223     -5.900 104.089  51.696  1.00 32.87      B   N
ATOM  3754  CA  ALA B 223     -5.895 105.466  51.201  1.00 36.60      B   C
ATOM  3755  CB  ALA B 223     -6.672 106.421  52.148  1.00 37.41      B   C
ATOM  3756  C   ALA B 223     -4.442 105.909  51.088  1.00 38.06      B   C
ATOM  3757  O   ALA B 223     -4.060 106.977  51.560  1.00 38.78      B   O
ATOM  3758  N   LEU B 224     -3.627 105.088  50.441  1.00 38.57      B   N
ATOM  3759  CA  LEU B 224     -2.215 105.403  50.264  1.00 38.61      B   C
ATOM  3760  CB  LEU B 224     -1.402 104.097  50.136  1.00 39.37      B   C
ATOM  3761  CG  LEU B 224     -1.183 103.355  51.466  1.00 39.96      B   C
ATOM  3762  CD1 LEU B 224     -0.057 102.350  51.297  1.00 39.16      B   C
ATOM  3763  CD2 LEU B 224     -0.818 104.336  52.585  1.00 41.79      B   C
ATOM  3764  C   LEU B 224     -1.949 106.306  49.064  1.00 38.91      B   C
ATOM  3765  O   LEU B 224     -2.714 106.190  48.105  1.00 38.22      B   O
ATOM  3766  OXT LEU B 224     -0.969 107.085  49.068  1.00 39.30      B   O
ATOM  3767  CB  PRO B 232     11.684 106.007  48.754  1.00 35.25      B   C
ATOM  3768  CG  PRO B 232     11.385 107.285  47.963  1.00 36.48      B   C
ATOM  3769  C   PRO B 232     13.583 105.559  50.328  1.00 32.21      B   C
ATOM  3770  O   PRO B 232     14.407 105.139  49.517  1.00 33.63      B   O
ATOM  3771  N   PRO B 232     13.132 107.820  49.423  1.00 34.70      B   N
ATOM  3772  CD  PRO B 232     12.673 108.108  48.053  1.00 35.80      B   C
ATOM  3773  CA  PRO B 232     12.514 106.559  49.903  1.00 34.68      B   C
ATOM  3774  N   LYS B 233     13.566 105.183  51.602  1.00 30.94      B   N
ATOM  3775  CA  LYS B 233     14.542 104.237  52.126  1.00 27.68      B   C
ATOM  3776  CB  LYS B 233     14.693 104.412  53.637  1.00 30.73      B   C
ATOM  3777  CG  LYS B 233     15.074 105.817  54.076  1.00 37.18      B   C
ATOM  3778  CD  LYS B 233     15.073 105.930  55.594  1.00 41.29      B   C
ATOM  3779  CE  LYS B 233     15.358 107.357  56.045  1.00 46.10      B   C
ATOM  3780  NZ  LYS B 233     15.389 107.476  57.535  1.00 49.46      B   N
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Figure 6OOO

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ATOM  3781  C   LYS B 233     14.115 102.805  51.823  1.00 25.78      B   C
ATOM  3782  O   LYS B 233     12.984 102.404  52.108  1.00 21.74      B   O
ATOM  3783  N   VAL B 234     15.027 102.041  51.238  1.00 23.23      B   N
ATOM  3784  CA  VAL B 234     14.755 100.652  50.902  1.00 22.01      B   C
ATOM  3785  CB  VAL B 234     14.425 100.486  49.403  1.00 22.47      B   C
ATOM  3786  CG1 VAL B 234     14.095  99.034  49.105  1.00 23.89      B   C
ATOM  3787  CG2 VAL B 234     13.267 101.386  49.015  1.00 24.31      B   C
ATOM  3788  C   VAL B 234     15.997  99.825  51.204  1.00 21.91      B   C
ATOM  3789  O   VAL B 234     17.083 100.121  50.702  1.00 19.49      B   O
ATOM  3790  N   GLU B 235     15.850  98.805  52.041  1.00 19.26      B   N
ATOM  3791  CA  GLU B 235     16.987  97.956  52.343  1.00 19.57      B   C
ATOM  3792  CB  GLU B 235     17.407  98.085  53.812  1.00 22.19      B   C
ATOM  3793  CG  GLU B 235     16.367  97.736  54.849  1.00 27.30      B   C
ATOM  3794  CD  GLU B 235     16.893  97.954  56.266  1.00 31.20      B   C
ATOM  3795  OE1 GLU B 235     17.214  99.113  56.617  1.00 30.91      B   O
ATOM  3796  OE2 GLU B 235     16.992  96.967  57.027  1.00 31.05      B   O
ATOM  3797  C   GLU B 235     16.667  96.513  51.979  1.00 17.90      B   C
ATOM  3798  O   GLU B 235     15.514  96.071  52.067  1.00 17.20      B   O
ATOM  3799  N   PHE B 236     17.694  95.797  51.538  1.00 15.16      B   N
ATOM  3800  CA  PHE B 236     17.540  94.417  51.121  1.00 14.57      B   C
ATOM  3801  CB  PHE B 236     18.080  94.240  49.702  1.00 13.24      B   C
ATOM  3802  CG  PHE B 236     17.406  95.123  48.695  1.00 14.78      B   C
ATOM  3803  CD1 PHE B 236     17.807  96.448  48.529  1.00 13.54      B   C
ATOM  3804  CD2 PHE B 236     16.338  94.647  47.944  1.00 13.10      B   C
ATOM  3805  CE1 PHE B 236     17.148  97.281  47.625  1.00 15.52      B   C
ATOM  3806  CE2 PHE B 236     15.676  95.471  47.043  1.00 11.79      B   C
ATOM  3807  CZ  PHE B 236     16.083  96.792  46.884  1.00 13.41      B   C
ATOM  3808  C   PHE B 236     18.206  93.432  52.055  1.00 14.79      B   C
ATOM  3809  O   PHE B 236     19.298  93.668  52.566  1.00 14.15      B   O
ATOM  3810  N   HIS B 237     17.519  92.319  52.270  1.00 13.68      B   N
ATOM  3811  CA  HIS B 237     17.993  91.266  53.147  1.00 11.28      B   C
ATOM  3812  CB  HIS B 237     17.235  91.319  54.466  1.00 12.27      B   C
ATOM  3813  CG  HIS B 237     17.437  92.597  55.219  1.00 14.02      B   C
ATOM  3814  CD2 HIS B 237     16.779  93.778  55.159  1.00 14.88      B   C
ATOM  3815  ND1 HIS B 237     18.460  92.771  56.126  1.00 14.41      B   N
ATOM  3816  CE1 HIS B 237     18.423  94.006  56.593  1.00 18.35      B   C
ATOM  3817  NE2 HIS B 237     17.413  94.638  56.023  1.00 14.90      B   N
ATOM  3818  C   HIS B 237     17.705  89.961  52.437  1.00 13.01      B   C
ATOM  3819  O   HIS B 237     16.725  89.860  51.702  1.00 12.07      B   O
ATOM  3820  N   ALA B 238     18.554  88.967  52.665  1.00 12.63      B   N
ATOM  3821  CA  ALA B 238     18.387  87.671  52.022  1.00 11.54      B   C
ATOM  3822  CB  ALA B 238     19.018  87.700  50.639  1.00  9.85      B   C
ATOM  3823  C   ALA B 238     19.010  86.554  52.836  1.00 14.48      B   C
ATOM  3824  O   ALA B 238     19.998  86.765  53.533  1.00 14.69      B   O
ATOM  3825  N   SER B 239     18.424  85.364  52.741  1.00 14.68      B   N
ATOM  3826  CA  SER B 239     18.948  84.202  53.447  1.00 14.80      B   C
ATOM  3827  CB  SER B 239     17.862  83.141  53.608  1.00 13.43      B   C
ATOM  3828  OG  SER B 239     17.340  82.758  52.355  1.00 13.26      B   O
ATOM  3829  C   SER B 239     20.104  83.656  52.614  1.00 14.91      B   C
ATOM  3830  O   SER B 239     20.945  82.902  53.107  1.00 12.99      B   O
ATOM  3831  N   GLY B 240     20.134  84.050  51.344  1.00 14.12      B   N
ATOM  3832  CA  GLY B 240     21.197  83.631  50.455  1.00 15.59      B   C
ATOM  3833  C   GLY B 240     22.217  84.752  50.346  1.00 16.66      B   C
ATOM  3834  O   GLY B 240     22.520  85.416  51.334  1.00 16.99      B   O
ATOM  3835  N   ASP B 241     22.732  84.985  49.145  1.00 15.94      B   N
ATOM  3836  CA  ASP B 241     23.722  86.036  48.947  1.00 17.18      B   C
ATOM  3837  CB  ASP B 241     24.487  85.795  47.649  1.00 18.32      B   C
ATOM  3838  CG  ASP B 241     25.703  86.673  47.527  1.00 21.73      B   C
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Figure 6PPP

ATOM 3839 OD1 ASP B 241 25.702 87.771 48.126 1.00 22.80 B O
ATOM 3840 OD2 ASP B 241 26.653 86.277 46.824 1.00 23.86 B O
ATOM 3841 C ASP B 241 23.070 87.416 48.899 1.00 15.91 B C
ATOM 3842 O ASP B 241 22.566 87.838 47.855 1.00 18.69 B O
ATOM 3843 N VAL B 242 23.091 88.125 50.022 1.00 15.82 B N
ATOM 3844 CA VAL B 242 22.480 89.447 50.079 1.00 15.47 B C
ATOM 3845 CB VAL B 242 22.373 89.961 51.538 1.00 14.55 B C
ATOM 3846 CG1 VAL B 242 23.753 90.329 52.079 1.00 14.67 B C
ATOM 3847 CG2 VAL B 242 21.405 91.147 51.599 1.00 13.95 B C
ATOM 3848 C VAL B 242 23.230 90.480 49.242 1.00 16.20 B C
ATOM 3849 O VAL B 242 22.624 91.396 48.693 1.00 16.97 B O
ATOM 3850 N ILE B 243 24.546 90.347 49.145 1.00 15.87 B N
ATOM 3851 CA ILE B 243 25.307 91.303 48.351 1.00 15.88 B C
ATOM 3852 CB ILE B 243 26.833 91.076 48.512 1.00 17.32 B C
ATOM 3853 CG2 ILE B 243 27.606 91.924 47.510 1.00 17.19 B C
ATOM 3854 CG1 ILE B 243 27.249 91.447 49.940 1.00 19.37 B C
ATOM 3855 CD1 ILE B 243 28.685 91.096 50.286 1.00 19.42 B C
ATOM 3856 C ILE B 243 24.882 91.191 46.889 1.00 14.23 B C
ATOM 3857 O ILE B 243 24.745 92.200 46.201 1.00 14.19 B O
ATOM 3858 N TRP B 244 24.651 89.967 46.421 1.00 14.60 B N
ATOM 3859 CA TRP B 244 24.207 89.756 45.046 1.00 14.98 B C
ATOM 3860 CB TRP B 244 24.078 88.264 44.729 1.00 15.60 B C
ATOM 3861 CG TRP B 244 23.575 87.999 43.329 1.00 16.65 B C
ATOM 3862 CD2 TRP B 244 22.210 87.806 42.930 1.00 19.35 B C
ATOM 3863 CE2 TRP B 244 22.206 87.617 41.527 1.00 18.45 B C
ATOM 3864 CE3 TRP B 244 20.989 87.775 43.622 1.00 18.90 B C
ATOM 3865 CD1 TRP B 244 24.321 87.924 42.184 1.00 18.57 B C
ATOM 3866 NE1 TRP B 244 23.506 87.694 41.097 1.00 17.92 B N
ATOM 3867 CZ2 TRP B 244 21.029 87.398 40.803 1.00 17.47 B C
ATOM 3868 CZ3 TRP B 244 19.818 87.558 42.902 1.00 18.34 B C
ATOM 3869 CH2 TRP B 244 19.847 87.371 41.504 1.00 17.51 B C
ATOM 3870 C TRP B 244 22.845 90.409 44.850 1.00 16.58 B C
ATOM 3871 O TRP B 244 22.616 91.102 43.859 1.00 17.56 B O
ATOM 3872 N LEU B 245 21.937 90.180 45.796 1.00 15.30 B N
ATOM 3873 CA LEU B 245 20.599 90.749 45.707 1.00 15.38 B C
ATOM 3874 CB LEU B 245 19.746 90.306 46.900 1.00 14.42 B C
ATOM 3875 CG LEU B 245 18.287 90.782 46.894 1.00 12.51 B C
ATOM 3876 CD1 LEU B 245 17.536 90.163 45.723 1.00 15.01 B C
ATOM 3877 CD2 LEU B 245 17.618 90.397 48.215 1.00 15.46 B C
ATOM 3878 C LEU B 245 20.648 92.270 45.660 1.00 15.93 B C
ATOM 3879 O LEU B 245 19.895 92.901 44.916 1.00 11.84 B O
ATOM 3880 N GLU B 246 21.534 92.865 46.454 1.00 16.60 B N
ATOM 3881 CA GLU B 246 21.636 94.317 46.480 1.00 17.29 B C
ATOM 3882 CB GLU B 246 22.496 94.782 47.658 1.00 18.17 B C
ATOM 3883 CG GLU B 246 21.896 94.455 49.020 1.00 19.87 B C
ATOM 3884 CD GLU B 246 22.776 94.908 50.176 1.00 21.82 B C
ATOM 3885 OE1 GLU B 246 24.001 94.687 50.101 1.00 23.59 B O
ATOM 3886 OE2 GLU B 246 22.244 95.471 51.161 1.00 18.84 B O
ATOM 3887 C GLU B 246 22.213 94.819 45.171 1.00 19.10 B C
ATOM 3888 O GLU B 246 21.866 95.905 44.711 1.00 18.10 B O
ATOM 3889 N ARG B 247 23.082 94.016 44.564 1.00 20.90 B N
ATOM 3890 CA ARG B 247 23.694 94.384 43.296 1.00 21.36 B C
ATOM 3891 CB ARG B 247 24.819 93.407 42.945 1.00 23.57 B C
ATOM 3892 CG ARG B 247 25.698 93.843 41.780 1.00 28.81 B C
ATOM 3893 CD ARG B 247 26.796 92.813 41.516 1.00 31.64 B C
ATOM 3894 NE ARG B 247 27.648 92.622 42.688 1.00 33.01 B N
ATOM 3895 CZ ARG B 247 27.953 91.437 43.214 1.00 34.15 B C
ATOM 3896 NH1 ARG B 247 27.475 90.319 42.678 1.00 32.31 B N

Figure 6QQQ

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ATOM  3897 NH2 ARG B 247     28.742  91.372  44.281  1.00 32.59    B   N
ATOM  3898 C   ARG B 247     22.612  94.369  42.218  1.00 21.28    B   C
ATOM  3899 O   ARG B 247     22.613  95.212  41.319  1.00 18.68    B   O
ATOM  3900 N   GLN B 248     21.689  93.411  42.316  1.00 19.88    B   N
ATOM  3901 CA  GLN B 248     20.587  93.310  41.359  1.00 18.33    B   C
ATOM  3902 CB  GLN B 248     19.778  92.027  41.586  1.00 16.87    B   C
ATOM  3903 CG  GLN B 248     20.458  90.749  41.119  1.00 17.30    B   C
ATOM  3904 CD  GLN B 248     20.794  90.768  39.631  1.00 21.87    B   C
ATOM  3905 OE1 GLN B 248     19.946  91.077  38.790  1.00 23.30    B   O
ATOM  3906 NE2 GLN B 248     22.032  90.423  39.304  1.00 24.03    B   N
ATOM  3907 C   GLN B 248     19.670  94.518  41.528  1.00 17.34    B   C
ATOM  3908 O   GLN B 248     19.166  95.071  40.550  1.00 16.87    B   O
ATOM  3909 N   ALA B 249     19.451  94.917  42.777  1.00 15.06    B   N
ATOM  3910 CA  ALA B 249     18.598  96.069  43.059  1.00 17.68    B   C
ATOM  3911 CB  ALA B 249     18.435  96.240  44.557  1.00 14.89    B   C
ATOM  3912 C   ALA B 249     19.210  97.332  42.449  1.00 16.19    B   C
ATOM  3913 O   ALA B 249     18.509  98.166  41.878  1.00 15.71    B   O
ATOM  3914 N   LYS B 250     20.523  97.466  42.578  1.00 15.67    B   N
ATOM  3915 CA  LYS B 250     21.221  98.625  42.039  1.00 16.75    B   C
ATOM  3916 CB  LYS B 250     22.686  98.599  42.493  1.00 20.71    B   C
ATOM  3917 CG  LYS B 250     23.555  99.725  41.952  1.00 24.70    B   C
ATOM  3918 CD  LYS B 250     23.089 101.093  42.425  1.00 29.48    B   C
ATOM  3919 CE  LYS B 250     24.028 102.180  41.914  1.00 34.06    B   C
ATOM  3920 NZ  LYS B 250     23.548 103.549  42.249  1.00 35.09    B   N
ATOM  3921 C   LYS B 250     21.137  98.633  40.514  1.00 16.02    B   C
ATOM  3922 O   LYS B 250     20.910  99.672  39.899  1.00 16.61    B   O
ATOM  3923 N   GLU B 251     21.300  97.464  39.907  1.00 16.92    B   N
ATOM  3924 CA  GLU B 251     21.256  97.366  38.457  1.00 16.87    B   C
ATOM  3925 CB  GLU B 251     21.789  96.009  38.000  1.00 17.15    B   C
ATOM  3926 CG  GLU B 251     21.913  95.902  36.492  1.00 19.76    B   C
ATOM  3927 CD  GLU B 251     22.195  94.495  36.030  1.00 21.03    B   C
ATOM  3928 OE1 GLU B 251     22.812  93.728  36.796  1.00 21.54    B   O
ATOM  3929 OE2 GLU B 251     21.813  94.159  34.891  1.00 23.50    B   O
ATOM  3930 C   GLU B 251     19.864  97.561  37.868  1.00 18.30    B   C
ATOM  3931 O   GLU B 251     19.696  98.297  36.895  1.00 18.23    B   O
ATOM  3932 N   TRP B 252     18.865  96.918  38.464  1.00 17.41    B   N
ATOM  3933 CA  TRP B 252     17.509  96.997  37.939  1.00 17.31    B   C
ATOM  3934 CB  TRP B 252     16.868  95.610  37.973  1.00 16.21    B   C
ATOM  3935 CG  TRP B 252     17.639  94.610  37.197  1.00 16.40    B   C
ATOM  3936 CD2 TRP B 252     17.650  94.459  35.775  1.00 17.43    B   C
ATOM  3937 CE2 TRP B 252     18.546  93.412  35.475  1.00 17.08    B   C
ATOM  3938 CE3 TRP B 252     16.988  95.107  34.723  1.00 20.12    B   C
ATOM  3939 CD1 TRP B 252     18.505  93.677  37.690  1.00 18.25    B   C
ATOM  3940 NE1 TRP B 252     19.053  92.954  36.662  1.00 17.57    B   N
ATOM  3941 CZ2 TRP B 252     18.799  92.996  34.167  1.00 16.27    B   C
ATOM  3942 CZ3 TRP B 252     17.239  94.691  33.416  1.00 18.36    B   C
ATOM  3943 CH2 TRP B 252     18.137  93.646  33.153  1.00 18.85    B   C
ATOM  3944 C   TRP B 252     16.555  98.000  38.565  1.00 20.68    B   C
ATOM  3945 O   TRP B 252     15.631  98.468  37.896  1.00 23.26    B   O
ATOM  3946 N   LEU B 253     16.762  98.333  39.833  1.00 20.19    B   N
ATOM  3947 CA  LEU B 253     15.878  99.279  40.508  1.00 22.15    B   C
ATOM  3948 CB  LEU B 253     15.392  98.680  41.832  1.00 19.99    B   C
ATOM  3949 CG  LEU B 253     14.796  97.269  41.748  1.00 20.08    B   C
ATOM  3950 CD1 LEU B 253     14.520  96.731  43.149  1.00 15.94    B   C
ATOM  3951 CD2 LEU B 253     13.521  97.299  40.918  1.00 20.16    B   C
ATOM  3952 C   LEU B 253     16.588 100.602  40.766  1.00 25.98    B   C
ATOM  3953 O   LEU B 253     15.971 101.573  41.213  1.00 28.88    B   O
ATOM  3954 N   LYS B 254     17.887 100.631  40.478  1.00 28.33    B   N
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Figure 6RRR

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ATOM  3955 CA  LYS B 254     18.713 101.822  40.684  1.00 32.00      B   C
ATOM  3956 CB  LYS B 254     18.210 102.985  39.818  1.00 33.97      B   C
ATOM  3957 CG  LYS B 254     17.844 102.597  38.388  1.00 37.77      B   C
ATOM  3958 CD  LYS B 254     18.983 101.890  37.661  1.00 38.80      B   C
ATOM  3959 CE  LYS B 254     18.544 101.453  36.265  1.00 41.63      B   C
ATOM  3960 NZ  LYS B 254     19.608 100.705  35.535  1.00 41.49      B   N
ATOM  3961 C   LYS B 254     18.677 102.214  42.162  1.00 32.29      B   C
ATOM  3962 O   LYS B 254     18.716 103.399  42.511  1.00 32.23      B   O
ATOM  3963 N   LEU B 255     18.603 101.201  43.022  1.00 31.24      B   N
ATOM  3964 CA  LEU B 255     18.560 101.397  44.469  1.00 34.52      B   C
ATOM  3965 CB  LEU B 255     17.250 100.844  45.039  1.00 34.04      B   C
ATOM  3966 CG  LEU B 255     15.917 101.437  44.584  1.00 36.59      B   C
ATOM  3967 CD1 LEU B 255     14.795 100.596  45.162  1.00 35.66      B   C
ATOM  3968 CD2 LEU B 255     15.791 102.888  45.036  1.00 36.85      B   C
ATOM  3969 C   LEU B 255     19.727 100.667  45.132  1.00 35.40      B   C
ATOM  3970 O   LEU B 255     20.326  99.794  44.473  1.00 34.56      B   O
ATOM  3971 OXT LEU B 255     20.014 100.959  46.310  1.00 38.02      B   O
ATOM  3972 N   GLD G 301     22.488  67.641  43.303  1.00  8.65      G   N
ATOM  3973 CA  GLD G 301     22.952  68.704  42.405  1.00 12.93      G   C
ATOM  3974 CB  GLD G 301     21.889  69.041  41.338  1.00 11.63      G   C
ATOM  3975 CG  GLD G 301     20.594  69.573  41.934  1.00 12.92      G   C
ATOM  3976 CD  GLD G 301     20.824  70.895  42.710  1.00 11.91      G   C
ATOM  3977 OE1 GLD G 301     21.256  71.889  42.077  1.00  9.76      G   O
ATOM  3978 OE2 GLD G 301     20.616  70.917  43.937  1.00 14.58      G   O
ATOM  3979 C   GLD G 301     24.267  68.360  41.735  1.00 11.46      G   C
ATOM  3980 O   GLD G 301     24.630  67.169  41.697  1.00 11.93      G   O
ATOM  3981 O1  GLD G 301     24.920  69.308  41.262  1.00 13.36      G   O
ATOM  3982 N   GLD H 302      8.053  83.746  43.978  1.00 11.84      H   N
ATOM  3983 CA  GLD H 302      7.425  82.601  43.310  1.00 14.35      H   C
ATOM  3984 CB  GLD H 302      8.287  82.089  42.143  1.00 12.93      H   C
ATOM  3985 CG  GLD H 302      9.638  81.579  42.619  1.00 15.67      H   C
ATOM  3986 CD  GLD H 302      9.448  80.386  43.597  1.00 14.81      H   C
ATOM  3987 OE1 GLD H 302      8.878  79.354  43.166  1.00 15.24      H   O
ATOM  3988 OE2 GLD H 302      9.825  80.506  44.780  1.00 14.34      H   O
ATOM  3989 C   GLD H 302      6.027  82.912  42.821  1.00 13.03      H   C
ATOM  3990 O   GLD H 302      5.676  84.098  42.749  1.00 11.51      H   O
ATOM  3991 O1  GLD H 302      5.308  81.938  42.528  1.00 15.43      H   O
ATOM  3992 C2  INH E  1     13.974  93.547  34.196  1.00 21.79      E   C
ATOM  3993 O11 INH E  1     13.261  94.464  33.777  1.00 21.09      E   O
ATOM  3994 N3  INH E  1     14.165  93.379  35.564  1.00 20.44      E   N
ATOM  3995 C7  INH E  1     13.557  94.278  36.569  1.00 20.49      E   C
ATOM  3996 C8  INH E  1     12.019  94.237  36.759  1.00 24.92      E   C
ATOM  3997 C10 INH E  1     11.708  94.941  38.091  1.00 25.12      E   C
ATOM  3998 C9  INH E  1     11.452  92.810  36.842  1.00 26.68      E   C
ATOM  3999 C4  INH E  1     14.957  92.363  36.018  1.00 19.38      E   C
ATOM  4000 N16 INH E  1     15.217  92.064  37.221  1.00 20.22      E   N
ATOM  4001 N15 INH E  1     16.020  90.988  37.236  1.00 18.99      E   N
ATOM  4002 C23 INH E  1     16.484  90.354  38.489  1.00 18.33      E   C
ATOM  4003 C24 INH E  1     15.792  88.946  38.541  1.00 19.18      E   C
ATOM  4004 C29 INH E  1     14.344  88.784  38.535  1.00 19.84      E   C
ATOM  4005 C30 INH E  1     13.446  89.896  38.512  1.00 20.83      E   C
ATOM  4006 C31 INH E  1     12.035  89.694  38.503  1.00 22.55      E   C
ATOM  4007 C32 INH E  1     11.503  88.377  38.513  1.00 24.46      E   C
ATOM  4008 C33 INH E  1     12.376  87.256  38.536  1.00 23.50      E   C
ATOM  4009 C28 INH E  1     13.783  87.448  38.549  1.00 21.97      E   C
ATOM  4010 C27 INH E  1     14.636  86.315  38.572  1.00 21.05      E   C
ATOM  4011 C26 INH E  1     16.045  86.483  38.584  1.00 19.47      E   C
ATOM  4012 C25 INH E  1     16.617  87.782  38.567  1.00 22.25      E   C
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Figure 6SSS

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ATOM  4013 C14 INH E   1      16.294  90.592  35.978  1.00 15.83      E   C
ATOM  4014 C17 INH E   1      17.178  89.405  35.585  1.00 16.67      E   C
ATOM  4015 C22 INH E   1      18.577  89.438  35.898  1.00 19.23      E   C
ATOM  4016 C21 INH E   1      19.395  88.340  35.554  1.00 18.31      E   C
ATOM  4017 N20 INH E   1      18.850  87.251  34.923  1.00 19.45      E   N
ATOM  4018 C19 INH E   1      17.516  87.188  34.607  1.00 18.95      E   C
ATOM  4019 C18 INH E   1      16.650  88.261  34.930  1.00 20.05      E   C
ATOM  4020 C5  INH E   1      15.629  91.408  35.147  1.00 16.08      E   C
ATOM  4021 C6  INH E   1      15.419  91.604  33.697  1.00 18.68      E   C
ATOM  4022 O13 INH E   1      15.959  90.832  32.910  1.00 18.22      E   O
ATOM  4023 N1  INH E   1      14.594  92.661  33.309  1.00 20.12      E   N
ATOM  4024 C12 INH E   1      14.373  92.853  31.870  1.00 19.38      E   C
ATOM  4025 C2  INH F   1      15.229  56.504  36.336  1.00 19.66      F   C
ATOM  4026 O11 INH F   1      15.872  55.553  35.883  1.00 19.27      F   O
ATOM  4027 N3  INH F   1      15.347  56.832  37.680  1.00 18.37      F   N
ATOM  4028 C7  INH F   1      16.244  56.066  38.574  1.00 21.01      F   C
ATOM  4029 C8  INH F   1      17.632  56.714  38.844  1.00 22.14      F   C
ATOM  4030 C10 INH F   1      18.576  56.443  37.657  1.00 27.02      F   C
ATOM  4031 C9  INH F   1      18.283  56.135  40.116  1.00 26.97      F   C
ATOM  4032 C4  INH F   1      14.636  57.891  38.181  1.00 20.15      F   C
ATOM  4033 N16 INH F   1      14.628  58.344  39.361  1.00 18.70      F   N
ATOM  4034 N15 INH F   1      13.787  59.404  39.418  1.00 20.10      F   N
ATOM  4035 C23 INH F   1      13.574  60.201  40.652  1.00 16.99      F   C
ATOM  4036 C24 INH F   1      14.177  61.615  40.365  1.00 16.25      F   C
ATOM  4037 C29 INH F   1      15.574  61.787  40.020  1.00 16.89      F   C
ATOM  4038 C30 INH F   1      16.491  60.678  39.950  1.00 17.51      F   C
ATOM  4039 C31 INH F   1      17.854  60.879  39.603  1.00 14.32      F   C
ATOM  4040 C32 INH F   1      18.324  62.192  39.315  1.00 19.70      F   C
ATOM  4041 C33 INH F   1      17.437  63.304  39.377  1.00 18.92      F   C
ATOM  4042 C28 INH F   1      16.071  63.112  39.727  1.00 19.84      F   C
ATOM  4043 C27 INH F   1      15.198  64.232  39.783  1.00 19.07      F   C
ATOM  4044 C26 INH F   1      13.829  64.056  40.129  1.00 19.02      F   C
ATOM  4045 C25 INH F   1      13.322  62.761  40.417  1.00 19.18      F   C
ATOM  4046 C14 INH F   1      13.224  59.615  38.219  1.00 20.53      F   C
ATOM  4047 C17 INH F   1      12.214  60.722  37.880  1.00 21.41      F   C
ATOM  4048 C22 INH F   1      10.902  60.683  38.443  1.00 24.07      F   C
ATOM  4049 C21 INH F   1       9.981  61.718  38.139  1.00 24.54      F   C
ATOM  4050 N20 INH F   1      10.356  62.748  37.310  1.00 24.94      F   N
ATOM  4051 C19 INH F   1      11.609  62.812  36.753  1.00 22.24      F   C
ATOM  4052 C18 INH F   1      12.564  61.805  37.024  1.00 22.59      F   C
ATOM  4053 C5  INH F   1      13.722  58.699  37.372  1.00 19.26      F   C
ATOM  4054 C6  INH F   1      13.620  58.311  35.947  1.00 19.59      F   C
ATOM  4055 O13 INH F   1      12.881  58.941  35.211  1.00 18.89      F   O
ATOM  4056 N1  INH F   1      14.371  57.239  35.521  1.00 18.86      F   N
ATOM  4057 C12 INH F   1      14.267  56.869  34.104  1.00 22.90      F   C
ATOM  4058 OH2 TIP S   1      26.694  70.185  39.535  1.00 10.43      S   O
ATOM  4059 OH2 TIP S   2      26.903  61.775  37.433  1.00 10.86      S   O
ATOM  4060 OH2 TIP S   3      35.118  64.928  45.661  1.00  9.77      S   O
ATOM  4061 OH2 TIP S   4       3.740  88.714  42.243  1.00 12.17      S   O
ATOM  4062 OH2 TIP S   5      -3.817  87.331  48.367  1.00 15.62      S   O
ATOM  4063 OH2 TIP S   6      16.515  80.411  54.861  1.00 15.64      S   O
ATOM  4064 OH2 TIP S   7      26.620  62.820  41.255  1.00 10.32      S   O
ATOM  4065 OH2 TIP S   8       3.173  81.112  41.277  1.00 12.87      S   O
ATOM  4066 OH2 TIP S   9      -5.009  77.145  39.859  1.00 14.54      S   O
ATOM  4067 OH2 TIP S  10      17.072  78.274  43.100  1.00 15.49      S   O
ATOM  4068 OH2 TIP S  11      11.094  82.014  54.953  1.00 13.66      S   O
ATOM  4069 OH2 TIP S  12      23.114  78.487  54.347  1.00 14.98      S   O
ATOM  4070 OH2 TIP S  13      20.046  86.513  47.218  1.00 13.55      S   O
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Figure 6TTT

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ATOM  4071 OH2 TIP S  14       2.655  89.017  38.291  1.00 15.07      S   O
ATOM  4072 OH2 TIP S  15       9.228  70.350  55.121  1.00 12.46      S   O
ATOM  4073 OH2 TIP S  16      16.739  84.862  44.381  1.00 12.76      S   O
ATOM  4074 OH2 TIP S  17      25.567  61.078  39.581  1.00 14.41      S   O
ATOM  4075 OH2 TIP S  18      37.252  56.626  40.690  1.00 14.19      S   O
ATOM  4076 OH2 TIP S  19      18.275  89.911  32.191  1.00 17.34      S   O
ATOM  4077 OH2 TIP S  20      34.008  72.385  38.024  1.00 14.04      S   O
ATOM  4078 OH2 TIP S  21      -1.688  79.172  55.257  1.00 19.38      S   O
ATOM  4079 OH2 TIP S  22      22.366  80.667  29.821  1.00 24.75      S   O
ATOM  4080 OH2 TIP S  23      12.380  75.091  59.029  1.00 20.05      S   O
ATOM  4081 OH2 TIP S  24      22.730  75.591  37.990  1.00 18.05      S   O
ATOM  4082 OH2 TIP S  25      -4.035  89.431  50.414  1.00 17.74      S   O
ATOM  4083 OH2 TIP S  26       4.573  89.940  39.949  1.00 14.11      S   O
ATOM  4084 OH2 TIP S  27      -1.906  87.737  40.180  1.00 17.43      S   O
ATOM  4085 OH2 TIP S  28      10.589  69.698  44.737  1.00 21.71      S   O
ATOM  4086 OH2 TIP S  29      25.201  95.439  52.148  1.00 16.83      S   O
ATOM  4087 OH2 TIP S  30      -8.367  85.700  23.246  1.00 15.98      S   O
ATOM  4088 OH2 TIP S  31      35.982  63.130  47.769  1.00 15.06      S   O
ATOM  4089 OH2 TIP S  32      21.296  70.481  54.804  1.00 19.30      S   O
ATOM  4090 OH2 TIP S  33      20.570  73.504  39.900  1.00 18.13      S   O
ATOM  4091 OH2 TIP S  34      27.666  49.772  40.587  1.00 14.52      S   O
ATOM  4092 OH2 TIP S  35       9.700  74.285  55.955  1.00 16.17      S   O
ATOM  4093 OH2 TIP S  36      12.186  64.800  48.529  1.00 17.60      S   O
ATOM  4094 OH2 TIP S  37      13.322  82.831  56.421  1.00 13.15      S   O
ATOM  4095 OH2 TIP S  38      34.693  38.751  49.392  1.00 20.67      S   O
ATOM  4096 OH2 TIP S  39      -5.001  91.649  54.454  1.00 20.34      S   O
ATOM  4097 OH2 TIP S  40      15.761  67.824  58.496  1.00 21.39      S   O
ATOM  4098 OH2 TIP S  41      11.148  84.424  43.877  1.00 12.67      S   O
ATOM  4099 OH2 TIP S  42      37.642  61.003  46.856  1.00 17.93      S   O
ATOM  4100 OH2 TIP S  43      -4.373  79.173  41.785  1.00 16.71      S   O
ATOM  4101 OH2 TIP S  44      43.723  52.077  51.584  1.00 18.94      S   O
ATOM  4102 OH2 TIP S  45      20.137  97.010  51.207  1.00 22.61      S   O
ATOM  4103 OH2 TIP S  46      -4.186  94.391  33.354  1.00 24.48      S   O
ATOM  4104 OH2 TIP S  47      10.434  59.744  34.860  1.00 20.09      S   O
ATOM  4105 OH2 TIP S  48      11.296  69.306  47.243  1.00 20.43      S   O
ATOM  4106 OH2 TIP S  49      13.514  84.678  43.033  1.00 17.25      S   O
ATOM  4107 OH2 TIP S  50      27.738  70.677  61.698  1.00 22.46      S   O
ATOM  4108 OH2 TIP S  51      16.289  72.356  55.129  1.00 13.74      S   O
ATOM  4109 OH2 TIP S  52      -4.477  95.904  37.489  1.00 27.31      S   O
ATOM  4110 OH2 TIP S  53      34.164  74.207  35.803  1.00 16.19      S   O
ATOM  4111 OH2 TIP S  54      13.181  73.070  43.734  1.00 17.17      S   O
ATOM  4112 OH2 TIP S  55      -3.958  90.260  57.512  1.00 25.11      S   O
ATOM  4113 OH2 TIP S  56      30.703  42.485  54.038  1.00 21.11      S   O
ATOM  4114 OH2 TIP S  57      30.922  56.349  27.885  1.00 20.13      S   O
ATOM  4115 OH2 TIP S  58      14.662  74.601  55.720  1.00 22.72      S   O
ATOM  4116 OH2 TIP S  59      38.507  59.138  50.812  1.00 19.14      S   O
ATOM  4117 OH2 TIP S  60      42.816  67.475  28.609  1.00 20.79      S   O
ATOM  4118 OH2 TIP S  61      -6.400  95.465  43.206  1.00 18.25      S   O
ATOM  4119 OH2 TIP S  62       6.561 102.864  47.606  1.00 21.89      S   O
ATOM  4120 OH2 TIP S  63      35.560  76.427  29.271  1.00 20.86      S   O
ATOM  4121 OH2 TIP S  64       5.810  69.019  32.123  1.00 25.31      S   O
ATOM  4122 OH2 TIP S  65      30.127  54.457  33.804  1.00 22.20      S   O
ATOM  4123 OH2 TIP S  66      14.517  98.509  59.915  1.00 20.97      S   O
ATOM  4124 OH2 TIP S  67      20.921  81.728  55.488  1.00 15.12      S   O
ATOM  4125 OH2 TIP S  68      18.125  78.127  55.061  1.00 22.38      S   O
ATOM  4126 OH2 TIP S  69       4.578 106.224  53.414  1.00 23.88      S   O
ATOM  4127 OH2 TIP S  70     -13.259  95.151  42.403  1.00 22.02      S   O
ATOM  4128 OH2 TIP S  71      19.506  66.848  43.948  1.00 14.64      S   O
```

Figure 6UUU

```
ATOM  4129  OH2 TIP S  72      20.492  58.168  29.357  1.00 24.23      S   O
ATOM  4130  OH2 TIP S  73      14.362  66.682  45.311  1.00 21.95      S   O
ATOM  4131  OH2 TIP S  74      37.948  64.500  49.199  1.00 22.89      S   O
ATOM  4132  OH2 TIP S  75      22.382  83.107  46.881  1.00 21.36      S   O
ATOM  4133  OH2 TIP S  76       2.257  71.707  33.743  1.00 22.26      S   O
ATOM  4134  OH2 TIP S  77      28.562  50.607  60.811  1.00 23.59      S   O
ATOM  4135  OH2 TIP S  78      12.908  55.269  54.605  1.00 22.04      S   O
ATOM  4136  OH2 TIP S  79      23.712  82.581  52.850  1.00 18.46      S   O
ATOM  4137  OH2 TIP S  80       6.000  64.702  50.376  1.00 22.24      S   O
ATOM  4138  OH2 TIP S  81      31.597  63.665  38.013  1.00 16.06      S   O
ATOM  4139  OH2 TIP S  82       3.204 101.393  39.851  1.00 18.09      S   O
ATOM  4140  OH2 TIP S  83      -3.695  88.746  62.013  1.00 24.84      S   O
ATOM  4141  OH2 TIP S  84      17.546  65.110  21.326  1.00 19.55      S   O
ATOM  4142  OH2 TIP S  85      26.824  59.347  62.759  1.00 26.30      S   O
ATOM  4143  OH2 TIP S  86      29.013  78.700  36.194  1.00 29.19      S   O
ATOM  4144  OH2 TIP S  87     -21.912  84.760  37.477  1.00 26.29      S   O
ATOM  4145  OH2 TIP S  88      37.659  49.564  54.905  1.00 21.54      S   O
ATOM  4146  OH2 TIP S  89      15.623  89.654  61.494  1.00 20.60      S   O
ATOM  4147  OH2 TIP S  90      46.913  73.636  27.864  1.00 24.09      S   O
ATOM  4148  OH2 TIP S  91      31.635  68.716  13.795  1.00 26.68      S   O
ATOM  4149  OH2 TIP S  92       8.998  77.444  41.106  1.00 21.52      S   O
ATOM  4150  OH2 TIP S  93      19.563  69.848  56.803  1.00 23.78      S   O
ATOM  4151  OH2 TIP S  94      21.054  77.796  57.903  1.00 20.91      S   O
ATOM  4152  OH2 TIP S  95      39.029  70.195  42.752  1.00 19.43      S   O
ATOM  4153  OH2 TIP S  96      16.357  59.879  28.472  1.00 34.72      S   O
ATOM  4154  OH2 TIP S  97       6.277  85.600  21.656  1.00 18.30      S   O
ATOM  4155  OH2 TIP S  98      24.381  79.010  25.797  1.00 24.45      S   O
ATOM  4156  OH2 TIP S  99      -0.330  73.515  46.326  1.00 21.44      S   O
ATOM  4157  OH2 TIP S 100      19.996  63.469  21.479  1.00 20.07      S   O
ATOM  4158  OH2 TIP S 101       8.484  64.804  37.057  1.00 21.03      S   O
ATOM  4159  OH2 TIP S 102      18.063  76.067  36.689  1.00 20.99      S   O
ATOM  4160  OH2 TIP S 103      13.804  68.104  43.044  1.00 25.16      S   O
ATOM  4161  OH2 TIP S 104      10.019  70.355  50.629  1.00 23.39      S   O
ATOM  4162  OH2 TIP S 105      36.764  63.450  55.390  1.00 19.23      S   O
ATOM  4163  OH2 TIP S 106      -3.017  81.106  52.043  1.00 29.08      S   O
ATOM  4164  OH2 TIP S 107      33.894  73.874  51.602  1.00 22.56      S   O
ATOM  4165  OH2 TIP S 108     -10.562  79.620  30.884  1.00 25.06      S   O
ATOM  4166  OH2 TIP S 109      -3.241  87.887  16.187  1.00 22.20      S   O
ATOM  4167  OH2 TIP S 110      36.320  79.997  40.961  1.00 30.47      S   O
ATOM  4168  OH2 TIP S 111      12.536  71.003  57.233  1.00 20.62      S   O
ATOM  4169  OH2 TIP S 112      -0.943  95.950  34.554  1.00 25.68      S   O
ATOM  4170  OH2 TIP S 113      14.938  45.779  46.539  1.00 32.69      S   O
ATOM  4171  OH2 TIP S 114      44.541  72.750  24.779  1.00 28.57      S   O
ATOM  4172  OH2 TIP S 115      16.028  56.338  61.884  1.00 27.69      S   O
ATOM  4173  OH2 TIP S 116      25.959  84.862  44.510  1.00 22.27      S   O
ATOM  4174  OH2 TIP S 117      11.898  70.641  40.303  1.00 29.38      S   O
ATOM  4175  OH2 TIP S 118      20.005  82.352  45.778  1.00 23.69      S   O
ATOM  4176  OH2 TIP S 119      24.653  82.113  42.509  1.00 26.73      S   O
ATOM  4177  OH2 TIP S 120      39.045  70.244  55.129  1.00 26.86      S   O
ATOM  4178  OH2 TIP S 121     -14.861  94.263  30.815  1.00 25.70      S   O
ATOM  4179  OH2 TIP S 122      28.805  79.348  55.384  1.00 24.42      S   O
ATOM  4180  OH2 TIP S 123      34.409  78.819  35.704  1.00 22.51      S   O
ATOM  4181  OH2 TIP S 124      25.708  95.887  48.431  1.00 22.52      S   O
ATOM  4182  OH2 TIP S 125      20.200  81.715  43.235  1.00 28.28      S   O
ATOM  4183  OH2 TIP S 126       8.358  89.545  27.306  1.00 25.44      S   O
ATOM  4184  OH2 TIP S 127      28.451  42.142  55.370  1.00 32.71      S   O
ATOM  4185  OH2 TIP S 128      -1.140  72.535  35.377  1.00 25.03      S   O
ATOM  4186  OH2 TIP S 129      42.723  73.261  29.197  1.00 26.01      S   O
```

Figure 6VVV

```
ATOM  4187  OH2 TIP S 130     0.475 106.754  43.565  1.00 35.60      S   O
ATOM  4188  OH2 TIP S 131    -8.799  81.517  47.238  1.00 30.82      S   O
ATOM  4189  OH2 TIP S 132    18.817  63.647  62.682  1.00 23.39      S   O
ATOM  4190  OH2 TIP S 133   -14.788  83.367  33.703  1.00 22.25      S   O
ATOM  4191  OH2 TIP S 134    28.486  47.289  40.587  1.00 26.04      S   O
ATOM  4192  OH2 TIP S 135    13.709  66.288  58.292  1.00 31.84      S   O
ATOM  4193  OH2 TIP S 136     4.869  72.011  43.934  1.00 21.85      S   O
ATOM  4194  OH2 TIP S 137   -19.103  77.442  35.205  1.00 29.80      S   O
ATOM  4195  OH2 TIP S 138    20.407  79.490  35.831  1.00 35.16      S   O
ATOM  4196  OH2 TIP S 139    10.860  84.010  22.443  1.00 27.02      S   O
ATOM  4197  OH2 TIP S 140     0.151 101.506  60.922  1.00 25.88      S   O
ATOM  4198  OH2 TIP S 141    31.584  47.279  41.254  1.00 23.80      S   O
ATOM  4199  OH2 TIP S 142    38.066  70.701  25.990  1.00 19.24      S   O
ATOM  4200  OH2 TIP S 143    44.977  72.631  31.204  1.00 23.78      S   O
ATOM  4201  OH2 TIP S 144    10.719  65.231  40.054  1.00 26.38      S   O
ATOM  4202  OH2 TIP S 145     7.475  91.297  29.034  1.00 27.02      S   O
ATOM  4203  OH2 TIP S 146    37.874  61.748  52.268  1.00 29.73      S   O
ATOM  4204  OH2 TIP S 147    -5.574  93.894  53.509  1.00 23.66      S   O
ATOM  4205  OH2 TIP S 148    17.820  78.905  36.654  1.00 28.79      S   O
ATOM  4206  OH2 TIP S 149    29.549  83.050  48.881  1.00 26.52      S   O
ATOM  4207  OH2 TIP S 150   -10.366 100.932  54.067  1.00 20.68      S   O
ATOM  4208  OH2 TIP S 151    30.504  64.646  60.794  1.00 28.37      S   O
ATOM  4209  OH2 TIP S 152    49.012  70.756  24.772  1.00 31.55      S   O
ATOM  4210  OH2 TIP S 153    30.846  45.257  57.188  1.00 31.72      S   O
ATOM  4211  OH2 TIP S 154    43.180  59.055  25.923  1.00 26.29      S   O
ATOM  4212  OH2 TIP S 155    22.523  66.585  65.647  1.00 32.96      S   O
ATOM  4213  OH2 TIP S 156     2.253 106.632  56.997  1.00 37.06      S   O
ATOM  4214  OH2 TIP S 157    21.987  90.927  36.214  1.00 24.25      S   O
ATOM  4215  OH2 TIP S 158    24.995  45.779  50.248  1.00 28.19      S   O
ATOM  4216  OH2 TIP S 159    24.701  87.274  52.417  1.00 25.41      S   O
ATOM  4217  OH2 TIP S 160    19.481  54.793  61.669  1.00 24.28      S   O
ATOM  4218  OH2 TIP S 161     5.052  66.267  52.559  1.00 20.50      S   O
ATOM  4219  OH2 TIP S 162    24.083  47.425  48.238  1.00 32.20      S   O
ATOM  4220  OH2 TIP S 163    50.567  67.161  31.028  1.00 21.83      S   O
ATOM  4221  OH2 TIP S 164    15.358  64.805  23.213  1.00 24.49      S   O
ATOM  4222  OH2 TIP S 165    -1.913  91.256  42.961  1.00 21.23      S   O
ATOM  4223  OH2 TIP S 166    32.576  60.552  40.991  1.00 24.61      S   O
ATOM  4224  OH2 TIP S 167     5.829  70.768  57.525  1.00 22.41      S   O
ATOM  4225  OH2 TIP S 168     6.357  83.074  62.946  1.00 20.77      S   O
ATOM  4226  OH2 TIP S 169    28.962  85.053  47.200  1.00 36.42      S   O
ATOM  4227  OH2 TIP S 170    22.828  55.785  37.965  1.00 34.04      S   O
ATOM  4228  OH2 TIP S 171     9.903 109.166  51.388  1.00 29.79      S   O
ATOM  4229  OH2 TIP S 172     6.629  71.093  33.592  1.00 24.39      S   O
ATOM  4230  OH2 TIP S 173    24.428  80.747  55.009  1.00 17.22      S   O
ATOM  4231  OH2 TIP S 174    11.049  67.896  25.243  1.00 28.73      S   O
ATOM  4232  OH2 TIP S 175    26.525  84.672  50.346  1.00 22.59      S   O
ATOM  4233  OH2 TIP S 176    14.485  79.387  59.276  1.00 36.33      S   O
ATOM  4234  OH2 TIP S 178    -8.133  88.350  22.930  1.00 24.98      S   O
ATOM  4235  OH2 TIP S 179    11.008  89.282  26.933  1.00 26.38      S   O
ATOM  4236  OH2 TIP S 180    29.198  77.232  57.047  1.00 28.34      S   O
ATOM  4237  OH2 TIP S 181    42.985  63.495  21.723  1.00 32.93      S   O
ATOM  4238  OH2 TIP S 182    -2.488  92.239  26.844  1.00 31.41      S   O
ATOM  4239  OH2 TIP S 183    38.070  68.391  49.950  1.00 27.44      S   O
ATOM  4240  OH2 TIP S 184     3.026  87.382  17.697  1.00 24.17      S   O
ATOM  4241  OH2 TIP S 185    32.032  45.265  50.288  1.00 26.40      S   O
ATOM  4242  OH2 TIP S 186    39.904  55.447  42.177  1.00 25.49      S   O
ATOM  4243  OH2 TIP S 187     2.867  70.555  28.600  1.00 25.55      S   O
ATOM  4244  OH2 TIP S 188    28.784  77.898  31.205  1.00 27.78      S   O
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Figure 6WWW

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ATOM  4245 OH2 TIP S 189      6.525  74.751  39.761  1.00 27.53      S   O
ATOM  4246 OH2 TIP S 190     -6.708  81.142  14.878  1.00 30.15      S   O
ATOM  4247 OH2 TIP S 191     23.949  87.249  38.410  1.00 26.94      S   O
ATOM  4248 OH2 TIP S 192      5.279  83.214  19.647  1.00 23.04      S   O
ATOM  4249 OH2 TIP S 193      7.787  93.915  65.832  1.00 34.56      S   O
ATOM  4250 OH2 TIP S 194     40.056  62.665  49.571  1.00 45.56      S   O
ATOM  4251 OH2 TIP S 195     17.005  83.158  42.309  1.00 26.09      S   O
ATOM  4252 OH2 TIP S 196     39.783  52.482  36.066  1.00 43.89      S   O
ATOM  4253 OH2 TIP S 197     21.034  85.408  34.631  1.00 21.18      S   O
ATOM  4254 OH2 TIP S 198     -2.760  93.994  35.518  1.00 32.71      S   O
ATOM  4255 OH2 TIP S 199    -14.876  77.201  34.781  1.00 29.91      S   O
ATOM  4256 OH2 TIP S 200      7.796  94.208  62.630  1.00 34.21      S   O
ATOM  4257 OH2 TIP S 201    -10.407  94.563  54.451  1.00 30.66      S   O
ATOM  4258 OH2 TIP S 202     19.132  85.088  38.251  1.00 26.36      S   O
ATOM  4259 OH2 TIP S 203     46.329  71.427  42.245  1.00 38.45      S   O
ATOM  4260 OH2 TIP S 204     38.151  49.728  42.054  1.00 23.90      S   O
ATOM  4261 OH2 TIP S 205    -16.881  92.357  37.722  1.00 29.19      S   O
ATOM  4262 OH2 TIP S 206      8.018  58.831  39.198  1.00 17.50      S   O
ATOM  4263 OH2 TIP S 207     23.689  77.990  32.612  1.00 37.51      S   O
ATOM  4264 OH2 TIP S 208     30.303  45.065  54.676  1.00 28.16      S   O
ATOM  4265 OH2 TIP S 209     25.161  84.823  52.568  1.00 29.69      S   O
ATOM  4266 OH2 TIP S 210     23.062  78.703  21.684  1.00 26.51      S   O
ATOM  4267 OH2 TIP S 211     26.355  47.512  59.226  1.00 41.38      S   O
ATOM  4268 OH2 TIP S 212     12.364  73.834  56.670  1.00 17.58      S   O
ATOM  4269 OH2 TIP S 213     22.789 101.251  38.634  1.00 36.48      S   O
ATOM  4270 OH2 TIP S 214     30.444  78.274  42.812  1.00 18.27      S   O
ATOM  4271 OH2 TIP S 215     16.714  66.636  43.404  1.00 27.82      S   O
ATOM  4272 OH2 TIP S 216     11.118 110.647  48.883  1.00 41.21      S   O
ATOM  4273 OH2 TIP S 217     11.938  77.223  62.477  1.00 26.78      S   O
ATOM  4274 OH2 TIP S 218     21.348  98.318  46.299  1.00 22.54      S   O
ATOM  4275 OH2 TIP S 219      6.335  90.109  61.055  1.00 30.93      S   O
ATOM  4276 OH2 TIP S 220     16.849  58.092  31.635  1.00 27.78      S   O
ATOM  4277 OH2 TIP S 221    -14.977  98.435  36.110  1.00 29.94      S   O
ATOM  4278 OH2 TIP S 222     32.209  56.644  34.417  1.00 27.61      S   O
ATOM  4279 OH2 TIP S 223     38.616  69.338  19.683  1.00 35.00      S   O
ATOM  4280 OH2 TIP S 224     43.793  66.187  40.980  1.00 28.57      S   O
ATOM  4281 OH2 TIP S 225     25.865  49.291  48.912  1.00 22.19      S   O
ATOM  4282 OH2 TIP S 226     29.493  51.282  39.294  1.00 28.59      S   O
ATOM  4283 OH2 TIP S 227      8.557  68.734  23.715  1.00 32.38      S   O
ATOM  4284 OH2 TIP S 228     35.030  72.215  49.061  1.00 21.47      S   O
ATOM  4285 OH2 TIP S 229     -5.863  84.407  53.693  1.00 32.71      S   O
ATOM  4286 OH2 TIP S 230      8.409  66.822  21.454  1.00 32.17      S   O
ATOM  4287 OH2 TIP S 231     16.090  88.535  25.766  1.00 45.41      S   O
ATOM  4288 OH2 TIP S 232      5.228  66.001  48.372  1.00 33.03      S   O
ATOM  4289 OH2 TIP S 233     22.372  81.334  39.929  1.00 38.56      S   O
ATOM  4290 OH2 TIP S 234    -11.344  82.468  23.312  1.00 32.37      S   O
ATOM  4291 OH2 TIP S 235     -5.663  88.297  52.367  1.00 28.46      S   O
ATOM  4292 OH2 TIP S 236     13.616  74.457  18.786  1.00 42.18      S   O
ATOM  4293 OH2 TIP S 237     25.283  53.133  37.923  1.00 40.56      S   O
ATOM  4294 OH2 TIP S 238      8.026  53.624  54.137  1.00 31.65      S   O
ATOM  4295 OH2 TIP S 239     34.534  62.367  11.800  1.00 31.60      S   O
ATOM  4296 OH2 TIP S 240      1.831  56.099  44.184  1.00 34.48      S   O
ATOM  4297 OH2 TIP S 241     49.497  62.599  26.810  1.00 26.78      S   O
ATOM  4298 OH2 TIP S 242     -4.758  72.368  21.533  1.00 38.11      S   O
ATOM  4299 OH2 TIP S 243     -5.868  83.431  58.623  1.00 34.40      S   O
ATOM  4300 OH2 TIP S 244     29.156  81.797  37.170  1.00 39.60      S   O
ATOM  4301 OH2 TIP S 245     21.609  85.611  37.638  1.00 20.34      S   O
ATOM  4302 OH2 TIP S 246     -4.284  77.490  49.709  1.00 35.30      S   O
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Figure 6XXX

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ATOM  4303  OH2 TIP S 247     31.807  48.664  61.432  1.00 43.66      S   O
ATOM  4304  OH2 TIP S 248     34.652  80.273  32.759  1.00 35.30      S   O
ATOM  4305  OH2 TIP S 249     -7.767  74.088  33.904  1.00 27.76      S   O
ATOM  4306  OH2 TIP S 250     -0.973  76.943  21.093  1.00 36.81      S   O
ATOM  4307  OH2 TIP S 251     17.520 103.841  50.759  1.00 37.13      S   O
ATOM  4308  OH2 TIP S 252     36.677  59.162  23.943  1.00 39.63      S   O
ATOM  4309  OH2 TIP S 253     -3.985  93.307  65.493  1.00 38.58      S   O
ATOM  4310  OH2 TIP S 254     26.053  53.836  34.851  1.00 37.31      S   O
ATOM  4311  OH2 TIP S 255     -7.010  78.156  28.377  1.00 28.40      S   O
ATOM  4312  OH2 TIP S 256      3.198  69.864  24.836  1.00 24.87      S   O
ATOM  4313  OH2 TIP S 257     -2.729  89.793  59.984  1.00 35.90      S   O
ATOM  4314  OH2 TIP S 259     12.874  62.780  21.486  1.00 40.71      S   O
ATOM  4315  OH2 TIP S 260     34.460  53.900  62.259  1.00 37.85      S   O
ATOM  4316  OH2 TIP S 261      8.524  50.114  40.677  1.00 29.93      S   O
ATOM  4317  OH2 TIP S 262     13.534  51.901  52.802  1.00 35.55      S   O
ATOM  4318  OH2 TIP S 263     -5.651  71.332  27.984  1.00 36.22      S   O
ATOM  4319  OH2 TIP S 264     10.884  74.117  37.648  1.00 23.87      S   O
ATOM  4320  OH2 TIP S 265      1.558 105.085  59.290  1.00 30.99      S   O
ATOM  4321  OH2 TIP S 267     22.855  87.241  54.244  1.00 39.85      S   O
ATOM  4322  OH2 TIP S 268     19.606  84.810  44.816  1.00 16.00      S   O
ATOM  4323  OH2 TIP S 269     10.246  57.810  32.854  1.00 25.86      S   O
ATOM  4324  OH2 TIP S 270    -21.599  79.618  39.328  1.00 38.76      S   O
ATOM  4325  OH2 TIP S 271     35.642  69.502  46.091  1.00 25.61      S   O
ATOM  4326  OH2 TIP S 272      7.124  71.606  39.935  1.00 32.52      S   O
ATOM  4327  OH2 TIP S 274     37.219  53.704  29.589  1.00 30.49      S   O
ATOM  4328  OH2 TIP S 275     15.688  71.656  41.660  1.00 35.47      S   O
ATOM  4329  OH2 TIP S 276     18.771  98.089  33.479  1.00 36.76      S   O
ATOM  4330  OH2 TIP S 277     18.891  96.723  59.037  1.00 34.81      S   O
ATOM  4331  OH2 TIP S 279     20.582  96.155  32.990  1.00 36.72      S   O
ATOM  4332  OH2 TIP S 280     38.382  46.507  54.083  1.00 22.09      S   O
ATOM  4333  OH2 TIP S 284     33.499  78.469  29.422  1.00 42.54      S   O
ATOM  4334  OH2 TIP S 285     43.663  56.107  27.511  1.00 34.42      S   O
ATOM  4335  OH2 TIP S 286     35.122  60.670  20.712  1.00 39.38      S   O
ATOM  4336  OH2 TIP S 287     -1.725  96.233  63.363  1.00 35.97      S   O
ATOM  4337  OH2 TIP S 290     18.717  83.949  40.601  1.00 23.89      S   O
ATOM  4338  OH2 TIP S 291     38.772  45.987  46.680  1.00 36.15      S   O
ATOM  4339  OH2 TIP S 292     20.224  69.382  59.695  1.00 29.64      S   O
ATOM  4340  OH2 TIP S 293      8.282  78.199  63.669  1.00 36.59      S   O
ATOM  4341  OH2 TIP S 294     14.047  63.860  59.319  1.00 44.69      S   O
ATOM  4342  OH2 TIP S 297     -5.817  72.739  40.818  1.00 38.14      S   O
ATOM  4343  OH2 TIP S 298     26.321  64.439  12.786  1.00 45.15      S   O
ATOM  4344  OH2 TIP S 299     -6.944 102.099  43.661  1.00 28.91      S   O
ATOM  4345  OH2 TIP S 300     31.982  51.444  38.891  1.00 26.30      S   O
ATOM  4346  OH2 TIP S 301     22.179  61.349  17.217  1.00 28.54      S   O
ATOM  4347  OH2 TIP S 302     11.846  66.672  46.440  1.00 15.33      S   O
ATOM  4348  OH2 TIP S 303     16.579  61.209  61.822  1.00 25.84      S   O
ATOM  4349  OH2 TIP S 304      9.179  61.102  31.089  1.00 35.18      S   O
ATOM  4350  OH2 TIP S 306     43.337  56.983  38.631  1.00 31.17      S   O
ATOM  4351  OH2 TIP S 307     -4.729  79.060  14.954  1.00 29.45      S   O
ATOM  4352  OH2 TIP S 309      3.264  96.531  34.343  1.00 35.87      S   O
ATOM  4353  OH2 TIP S 310     33.597  56.115  32.020  1.00 38.28      S   O
ATOM  4354  OH2 TIP S 312     21.131  84.199  42.642  1.00 16.36      S   O
ATOM  4355  OH2 TIP S 314     13.289  90.298  22.035  1.00 37.86      S   O
ATOM  4356  OH2 TIP S 315    -21.318  88.597  32.650  1.00 31.68      S   O
ATOM  4357  OH2 TIP S 316      0.324  97.812  61.903  1.00 28.65      S   O
ATOM  4358  OH2 TIP S 317     15.681  48.773  53.561  1.00 32.11      S   O
ATOM  4359  OH2 TIP S 318      6.414  66.203  28.644  1.00 45.39      S   O
ATOM  4360  OH2 TIP S 320     21.877  45.789  57.051  1.00 37.88      S   O
```

Figure 6YYY

```
ATOM  4361  OH2 TIP S 325      33.257  76.751  48.828  1.00 36.69      S   O
ATOM  4362  OH2 TIP S 326      -1.477  99.714  39.504  1.00 31.96      S   O
ATOM  4363  OH2 TIP S 327       7.083 107.442  40.232  1.00 34.50      S   O
ATOM  4364  OH2 TIP S 328      19.455  81.284  39.450  1.00 31.13      S   O
ATOM  4365  OH2 TIP S 330      18.928  59.678  27.698  1.00 23.64      S   O
ATOM  4366  OH2 TIP S 333       2.949  68.265  43.594  1.00 46.66      S   O
ATOM  4367  OH2 TIP S 334      -8.138 104.339  45.239  1.00 36.83      S   O
ATOM  4368  OH2 TIP S 336       3.891  58.458  48.159  1.00 40.09      S   O
ATOM  4369  OH2 TIP S 339     -11.491  79.098  22.692  1.00 31.58      S   O
ATOM  4370  OH2 TIP S 342      -3.605  77.350  56.479  1.00 33.40      S   O
ATOM  4371  OH2 TIP S 345      48.945  64.149  23.906  1.00 33.98      S   O
ATOM  4372  OH2 TIP S 348      17.597  50.879  59.000  1.00 46.70      S   O
ATOM  4373  OH2 TIP S 349     -19.548  99.216  33.850  1.00 31.30      S   O
ATOM  4374  OH2 TIP S 350      11.566  66.969  42.047  1.00 25.33      S   O
ATOM  4375  OH2 TIP S 353      24.674  43.379  42.738  1.00 46.49      S   O
ATOM  4376  OH2 TIP S 354      20.654  78.836  55.418  1.00 19.53      S   O
ATOM  4377  OH2 TIP S 357      17.254  91.782  60.031  1.00 23.92      S   O
ATOM  4378  OH2 TIP S 358       9.923  67.047  44.491  1.00 20.59      S   O
ATOM  4379  OH2 TIP S 359      36.952  66.998  45.661  1.00 21.28      S   O
ATOM  4380  OH2 TIP S 360      15.012  70.447  58.501  1.00 20.49      S   O
ATOM  4381  OH2 TIP S 361      38.560  66.828  47.799  1.00 18.16      S   O
ATOM  4382  OH2 TIP S 362      12.567  70.351  43.331  1.00 21.60      S   O
ATOM  4383  OH2 TIP S 363      10.275  70.909  59.173  1.00 20.25      S   O
ATOM  4384  OH2 TIP S 365      -8.636  80.604  29.420  1.00 20.84      S   O
ATOM  4385  OH2 TIP S 366      27.535  82.312  43.508  1.00 25.30      S   O
ATOM  4386  OH2 TIP S 367      17.257  86.397  26.338  1.00 29.08      S   O
ATOM  4387  OH2 TIP S 368       4.358  55.280  44.796  1.00 40.14      S   O
ATOM  4388  OH2 TIP S 369       8.463  83.561  21.334  1.00 22.41      S   O
ATOM  4389  OH2 TIP S 370      -8.086  97.612  37.816  1.00 25.46      S   O
ATOM  4390  OH2 TIP S 371      12.843  74.928  39.116  1.00 31.70      S   O
ATOM  4391  OH2 TIP S 372       8.347  72.232  57.105  1.00 25.70      S   O
ATOM  4392  OH2 TIP S 373      -3.834 109.911  52.412  1.00 25.46      S   O
ATOM  4393  OH2 TIP S 374      38.734  67.042  43.751  1.00 25.21      S   O
ATOM  4394  OH2 TIP S 375      20.952  90.132  33.041  1.00 26.25      S   O
ATOM  4395  OH2 TIP S 376      21.122  98.404  49.083  1.00 21.33      S   O
ATOM  4396  OH2 TIP S 377     -12.795  97.771  42.948  1.00 27.19      S   O
ATOM  4397  OH2 TIP S 378      24.316  79.549  28.534  1.00 25.40      S   O
ATOM  4398  OH2 TIP S 379      27.736  88.375  45.434  1.00 29.24      S   O
ATOM  4399  OH2 TIP S 380       8.225  59.683  36.172  1.00 24.77      S   O
ATOM  4400  OH2 TIP S 381      37.450  53.227  35.003  1.00 32.48      S   O
ATOM  4401  OH2 TIP S 382     -10.586  84.900  22.199  1.00 30.47      S   O
ATOM  4402  OH2 TIP S 383     -15.137  95.854  40.707  1.00 25.76      S   O
ATOM  4403  OH2 TIP S 384      16.777  65.477  62.229  1.00 26.46      S   O
ATOM  4404  OH2 TIP S 385      28.839  86.168  50.617  1.00 33.26      S   O
ATOM  4405  OH2 TIP S 386      17.382  84.892  57.199  1.00 22.87      S   O
ATOM  4406  OH2 TIP S 387      27.000  52.190  62.926  1.00 27.15      S   O
ATOM  4407  OH2 TIP S 388      31.661  79.835  35.615  1.00 28.03      S   O
ATOM  4408  OH2 TIP S 389      -4.676  84.758  48.894  1.00 31.68      S   O
ATOM  4409  OH2 TIP S 390      -5.662  91.557  50.040  1.00 31.19      S   O
ATOM  4410  OH2 TIP S 391      23.487  83.965  44.473  1.00 28.65      S   O
ATOM  4411  OH2 TIP S 392      -6.441  88.875  58.175  1.00 33.33      S   O
ATOM  4412  OH2 TIP S 393       7.603  93.526  36.250  1.00 30.57      S   O
ATOM  4413  OH2 TIP S 394      49.203  72.825  26.301  1.00 24.46      S   O
ATOM  4414  OH2 TIP S 395      28.479  61.371  62.617  1.00 32.12      S   O
ATOM  4415  OH2 TIP S 397      -9.168  83.076  17.253  1.00 25.74      S   O
ATOM  4416  OH2 TIP S 398      16.075  88.965  63.990  1.00 30.49      S   O
ATOM  4417  OH2 TIP S 400      13.310  95.842  67.259  1.00 29.76      S   O
ATOM  4418  OH2 TIP S 401       5.918  66.938  33.592  1.00 31.14      S   O
```

Figure 6ZZZ

```
ATOM  4419  OH2 TIP S 402      0.155 106.248  55.777  1.00 32.60      S   O
ATOM  4420  OH2 TIP S 403      6.110  92.248  62.655  1.00 27.95      S   O
ATOM  4421  OH2 TIP S 404      2.233 103.880  39.763  1.00 31.52      S   O
ATOM  4422  OH2 TIP S 405     25.694  98.715  48.972  1.00 29.93      S   O
ATOM  4423  OH2 TIP S 406     10.674  73.231  60.407  1.00 31.34      S   O
ATOM  4424  OH2 TIP S 409     51.882  66.157  29.120  1.00 26.96      S   O
ATOM  4425  OH2 TIP S 410      6.325  68.647  46.053  1.00 34.29      S   O
ATOM  4426  OH2 TIP S 412     39.391  64.285  54.825  1.00 28.64      S   O
ATOM  4427  OH2 TIP S 413     -2.620  73.079  47.858  1.00 31.55      S   O
ATOM  4428  OH2 TIP S 414     32.879  78.973  43.464  1.00 29.58      S   O
ATOM  4429  OH2 TIP S 415    -15.016  96.572  33.202  1.00 45.53      S   O
ATOM  4430  OH2 TIP S 416     39.377  75.743  32.551  1.00 30.17      S   O
ATOM  4431  OH2 TIP S 417     31.294  47.074  59.585  1.00 32.29      S   O
ATOM  4432  OH2 TIP S 418     20.908  99.085  60.072  1.00 33.84      S   O
ATOM  4433  OH2 TIP S 421     16.227  75.089  58.255  1.00 34.63      S   O
ATOM  4434  OH2 TIP S 423      9.515  68.766  41.162  1.00 31.09      S   O
ATOM  4435  OH2 TIP S 424     24.057  90.877  41.184  1.00 32.57      S   O
ATOM  4436  OH2 TIP S 425    -23.421  85.321  34.874  1.00 40.73      S   O
ATOM  4437  OH2 TIP S 426     -6.600  85.509  60.637  1.00 36.33      S   O
ATOM  4438  OH2 TIP S 429     18.068  74.274  39.152  1.00 28.30      S   O
ATOM  4439  OH2 TIP S 430      0.216  72.088  29.280  1.00 34.77      S   O
ATOM  4440  OH2 TIP S 431     24.237  97.970  52.510  1.00 40.38      S   O
ATOM  4441  OH2 TIP S 433     16.496  61.776  20.380  1.00 31.74      S   O
ATOM  4442  OH2 TIP S 434     23.656  81.140  23.402  1.00 39.14      S   O
ATOM  4443  OH2 TIP S 435     45.512  70.376  23.767  1.00 38.06      S   O
ATOM  4444  OH2 TIP S 436      5.133  69.622  42.446  1.00 33.04      S   O
ATOM  4445  OH2 TIP S 440     23.692  79.457  34.661  1.00 40.65      S   O
ATOM  4446  OH2 TIP S 443     15.889  73.328  39.832  1.00 29.37      S   O
ATOM  4447  OH2 TIP S 444     -8.745  70.532  28.410  1.00 33.62      S   O
ATOM  4448  OH2 TIP S 446     32.260  78.506  13.999  1.00 45.13      S   O
ATOM  4449  OH2 TIP S 448     39.242  48.079  43.803  1.00 33.38      S   O
ATOM  4450  OH2 TIP S 449     34.559  75.768  22.405  1.00 31.84      S   O
ATOM  4451  OH2 TIP S 450     17.344  71.627  57.656  1.00 30.16      S   O
ATOM  4452  OH2 TIP S 453     17.850  55.704  64.074  1.00 41.95      S   O
ATOM  4453  OH2 TIP S 454     12.673  87.630  65.105  1.00 36.77      S   O
ATOM  4454  OH2 TIP S 455     18.393  73.689  58.998  1.00 35.69      S   O
ATOM  4455  OH2 TIP S 457     31.350  80.284  54.849  1.00 32.98      S   O
ATOM  4456  OH2 TIP S 459     31.948  64.117  63.134  1.00 33.16      S   O
ATOM  4457  OH2 TIP S 461     25.883  44.584  58.922  1.00 26.81      S   O
ATOM  4458  OH2 TIP S 462     15.411  75.744  38.970  1.00 38.18      S   O
ATOM  4459  OH2 TIP S 465     -6.694  85.996  51.462  1.00 39.03      S   O
ATOM  4460  OH2 TIP S 467     22.428  74.991  56.119  1.00 48.69      S   O
ATOM  4461  OH2 TIP S 472      7.409  68.343  43.765  1.00 40.63      S   O
ATOM  4462  OH2 TIP S 477      3.696  81.760  15.765  1.00 41.18      S   O
ATOM  4463  OH2 TIP S 478     36.353  75.696  51.865  1.00 40.40      S   O
ATOM  4464  OH2 TIP S 479     45.063  73.009  39.613  1.00 30.28      S   O
ATOM  4465  OH2 TIP S 480     35.167  68.155  64.949  1.00 36.43      S   O
ATOM  4466  OH2 TIP S 481     16.895  81.810  19.179  1.00 26.87      S   O
ATOM  4467  OH2 TIP S 482      9.338  64.581  19.670  1.00 47.45      S   O
ATOM  4468  OH2 TIP S 486     -4.142  97.143  32.076  1.00 40.89      S   O
ATOM  4469  OH2 TIP S 492      8.626 110.626  48.140  1.00 38.81      S   O
ATOM  4470  OH2 TIP S 493     10.344  52.396  54.552  1.00 40.72      S   O
ATOM  4471  OH2 TIP S 504     -6.927  90.936  52.736  1.00 32.58      S   O
ATOM  4472  OH2 TIP S 506     25.842  56.111  26.259  1.00 44.04      S   O
ATOM  4473  OH2 TIP S 511    -18.765  81.021  30.433  1.00 43.07      S   O
ATOM  4474  OH2 TIP S 514    -10.951  95.897  30.634  1.00 35.08      S   O
ATOM  4475  OH2 TIP S 515     18.239  91.555  29.988  1.00 35.01      S   O
ATOM  4476  OH2 TIP S 518     11.487  71.453  37.559  1.00 30.35      S   O
```

Figure 6AAAA

```
ATOM  4477  OH2 TIP S 519     -5.621  94.181  63.866  1.00 38.29      S   O
ATOM  4478  OH2 TIP S 522    -22.715  82.630  39.313  1.00 37.68      S   O
ATOM  4479  OH2 TIP S 523     13.832  92.634  28.634  1.00 42.35      S   O
ATOM  4480  OH2 TIP S 526     38.684  51.235  34.304  1.00 47.63      S   O
ATOM  4481  OH2 TIP S 528     36.575  81.337  36.652  1.00 30.20      S   O
ATOM  4482  OH2 TIP S 529     19.003  94.626  60.449  1.00 33.39      S   O
ATOM  4483  OH2 TIP S 532     45.213  64.758  44.484  1.00 43.40      S   O
ATOM  4484  OH2 TIP S 548     27.913  76.880  61.466  1.00 39.53      S   O
ATOM  4485  OH2 TIP S 550     -7.794  83.071  55.228  1.00 36.58      S   O
ATOM  4486  OH2 TIP S 551      6.856  87.791  20.410  1.00 45.36      S   O
ATOM  4487  OH2 TIP S 553     20.954  56.587  35.076  1.00 46.06      S   O
ATOM  4488  OH2 TIP S 559      6.709  95.476  37.577  1.00 37.67      S   O
ATOM  4489  OH2 TIP S 561     -5.111  70.585  43.095  1.00 36.29      S   O
ATOM  4490  OH2 TIP S 563     33.592  49.188  39.439  1.00 38.90      S   O
ATOM  4491  OH2 TIP S 567     24.268  93.456  38.866  1.00 41.73      S   O
ATOM  4492  OH2 TIP S 568     38.145  71.373  18.079  1.00 45.93      S   O
ATOM  4493  OH2 TIP S 570     10.042 104.897  57.893  1.00 35.94      S   O
ATOM  4494  OH2 TIP S 579      2.980  71.667  46.083  1.00 31.08      S   O
ATOM  4495  OH2 TIP S 588     42.992  48.494  46.292  1.00 42.53      S   O
ATOM  4496  OH2 TIP S 592      7.979 101.256  62.776  1.00 43.56      S   O
ATOM  4497  OH2 TIP S 596     40.729  51.604  40.374  1.00 44.86      S   O
ATOM  4498  OH2 TIP S 608     22.066  82.819  34.739  1.00 44.19      S   O
ATOM  4499  OH2 TIP S 612     23.253  56.890  32.646  1.00 37.91      S   O
ATOM  4500  OH2 TIP S 613     -4.126  71.281  39.257  1.00 40.53      S   O
ATOM  4501  OH2 TIP S 640     21.624 103.517  40.110  1.00 37.27      S   O
ATOM  4502  OH2 TIP S 648      5.614  70.703  52.258  1.00 52.65      S   O
ATOM  4503  OH2 TIP S 650     43.903  58.744  50.765  1.00 33.40      S   O
ATOM  4504  OH2 TIP S 655     -8.816  78.637  48.006  1.00 40.13      S   O
ATOM  4505  OH2 TIP S 656     -5.358  78.170  23.376  1.00 32.77      S   O
ATOM  4506  OH2 TIP S 657      3.160  70.067  31.591  1.00 35.22      S   O
ATOM  4507  OH2 TIP S 658     25.185  73.553  62.291  1.00 39.81      S   O
END
```

Figure 7A

```
REMARK Created by MOLEMAN V. 991230/7.3 at Tue Dec 10 19:34:52 2002 for kemitl
REMARK MoleMan PDB file
REMARK Created by MOLEMAN V. 961218/7.2.5 at Tue Mar 28 15:09:11 2000 for kemitl
REMARK MoleMan PDB file
REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 1.86 A
REMARK starting r= 0.2208 free_r= 0.2457
REMARK final   r= 0.2055 free_r= 0.2376
REMARK B rmsd for bonded mainchain atoms=  1.483  target= 1.5
REMARK B rmsd for bonded sidechain atoms=  2.506  target= 2.0
REMARK B rmsd for angle mainchain atoms=  2.042  target= 2.0
REMARK B rmsd for angle sidechain atoms=  3.617  target= 2.5
REMARK wa= 1.64705
REMARK rweight=6.377507E-02
REMARK target= mlf  steps= 50
REMARK sg= P2(1)2(1)2(1) a= 61.41 b= 76.31 c= 108.92 alpha= 90 beta= 90 gamma= 90
REMARK parameter file 1  : MSI_CNX_TOPPAR:protein_rep.param
REMARK parameter file 2  : MSI_CNX_TOPPAR:water_rep.param
REMARK parameter file 3  : inh.par
REMARK parameter file 4  : gld.par
REMARK molecular structure file: generate_easy.psf
REMARK input coordinates: bgroup.pdb
REMARK reflection file= muri_1.8.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.86
REMARK initial B-factor correction applied to fobs :
REMARK   B11=   0.497 B22=   1.667 B33=  -2.164
REMARK   B12=   0.000 B13=   0.000 B23=   0.000
REMARK B-factor correction applied to coordinate array B:    1.176
REMARK bulk solvent: (Mask) density level= 0.365438 e/A^3, B-factor= 33.2255 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range:    43743 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):  3410 (  7.8 % )
REMARK number of reflections rejected:                           0 (  0.0 % )
REMARK total number of reflections used:                     40333 ( 92.2 % )
REMARK number of reflections in working set:                 38313 ( 87.6 % )
REMARK number of reflections in test set:                     2020 (  4.6 % )
REMARK FILENAME="bindividual.pdb"
REMARK DATE:Mar-24-2000  16:16:02      created by user: kemitl
REMARK Written by CNX VERSION:2000
CRYST1  61.410  76.310 108.920  90.00  90.00  90.00 P212121      1
ORIGX1    1.000000  0.000000  0.000000        0.00000
ORIGX2    0.000000  1.000000  0.000000        0.00000
ORIGX3    0.000000  0.000000  1.000000        0.00000
SCALE1    0.016284  0.000000  0.000000        0.00000
SCALE2    0.000000  0.013104  0.000000        0.00000
SCALE3    0.000000  0.000000  0.009181        0.00000
ATOM      1  CB  MET A   1      30.124  48.907  56.585  1.00 22.42      A   C
ATOM      2  CG  MET A   1      30.702  50.302  56.333  1.00 25.22      A   C
ATOM      3  SD  MET A   1      31.489  51.055  57.785  1.00 28.98      A   S
ATOM      4  CE  MET A   1      32.951  49.983  58.010  1.00 26.14      A   C
ATOM      5  C   MET A   1      27.890  49.690  57.412  1.00 19.35      A   C
ATOM      6  O   MET A   1      27.114  49.386  56.503  1.00 20.53      A   O
ATOM      7  N   MET A   1      28.658  47.421  57.925  1.00 18.28      A   N
ATOM      8  CA  MET A   1      29.106  48.829  57.729  1.00 20.61      A   C
ATOM      9  N   LYS A   2      27.729  50.760  58.178  1.00 18.84      A   N
ATOM     10  CA  LYS A   2      26.605  51.666  58.005  1.00 19.29      A   C
```

Figure 7B

```
ATOM   11 CB  LYS A  2    25.834  51.769  59.316  1.00 18.82    A   C
ATOM   12 CG  LYS A  2    24.636  52.702  59.295  1.00 20.09    A   C
ATOM   13 CD  LYS A  2    24.005  52.752  60.674  1.00 22.85    A   C
ATOM   14 CE  LYS A  2    22.697  53.523  60.676  1.00 22.98    A   C
ATOM   15 NZ  LYS A  2    22.078  53.501  62.033  1.00 22.51    A   N
ATOM   16 C   LYS A  2    27.131  53.031  57.588  1.00 17.25    A   C
ATOM   17 O   LYS A  2    27.980  53.616  58.265  1.00 16.44    A   O
ATOM   18 N   ILE A  3    26.630  53.533  56.464  1.00 17.70    A   N
ATOM   19 CA  ILE A  3    27.075  54.824  55.968  1.00 14.65    A   C
ATOM   20 CB  ILE A  3    28.001  54.647  54.738  1.00 16.82    A   C
ATOM   21 CG2 ILE A  3    29.214  53.807  55.121  1.00 17.12    A   C
ATOM   22 CG1 ILE A  3    27.252  53.971  53.593  1.00 17.27    A   C
ATOM   23 CD1 ILE A  3    26.697  54.929  52.583  1.00 20.09    A   C
ATOM   24 C   ILE A  3    25.925  55.758  55.617  1.00 14.64    A   C
ATOM   25 O   ILE A  3    24.752  55.377  55.639  1.00 14.39    A   O
ATOM   26 N   GLY A  4    26.269  57.001  55.322  1.00 13.89    A   N
ATOM   27 CA  GLY A  4    25.244  57.956  54.961  1.00 14.96    A   C
ATOM   28 C   GLY A  4    25.500  58.490  53.569  1.00 13.26    A   C
ATOM   29 O   GLY A  4    26.634  58.453  53.081  1.00 11.89    A   O
ATOM   30 N   VAL A  5    24.439  58.954  52.917  1.00 11.22    A   N
ATOM   31 CA  VAL A  5    24.549  59.541  51.592  1.00 10.79    A   C
ATOM   32 CB  VAL A  5    23.964  58.625  50.500  1.00 14.07    A   C
ATOM   33 CG1 VAL A  5    23.918  59.363  49.169  1.00 12.77    A   C
ATOM   34 CG2 VAL A  5    24.828  57.385  50.352  1.00 12.02    A   C
ATOM   35 C   VAL A  5    23.771  60.848  51.643  1.00 11.63    A   C
ATOM   36 O   VAL A  5    22.596  60.872  52.020  1.00 12.22    A   O
ATOM   37 N   PHE A  6    24.445  61.932  51.287  1.00 11.51    A   N
ATOM   38 CA  PHE A  6    23.848  63.256  51.302  1.00 13.29    A   C
ATOM   39 CB  PHE A  6    24.674  64.182  52.203  1.00 13.43    A   C
ATOM   40 CG  PHE A  6    24.252  65.620  52.143  1.00 14.85    A   C
ATOM   41 CD1 PHE A  6    22.937  65.981  52.418  1.00 16.29    A   C
ATOM   42 CD2 PHE A  6    25.164  66.612  51.800  1.00 15.26    A   C
ATOM   43 CE1 PHE A  6    22.530  67.317  52.350  1.00 17.43    A   C
ATOM   44 CE2 PHE A  6    24.770  67.954  51.728  1.00 17.55    A   C
ATOM   45 CZ  PHE A  6    23.450  68.305  52.003  1.00 18.07    A   C
ATOM   46 C   PHE A  6    23.725  63.887  49.920  1.00 12.87    A   C
ATOM   47 O   PHE A  6    24.641  63.806  49.102  1.00 14.09    A   O
ATOM   48 N   ASP A  7    22.583  64.519  49.674  1.00 11.45    A   N
ATOM   49 CA  ASP A  7    22.331  65.212  48.418  1.00 12.53    A   C
ATOM   50 CB  ASP A  7    21.749  64.263  47.363  1.00 11.52    A   C
ATOM   51 CG  ASP A  7    21.491  64.959  46.035  1.00 10.71    A   C
ATOM   52 OD1 ASP A  7    22.444  65.525  45.457  1.00 12.13    A   O
ATOM   53 OD2 ASP A  7    20.332  64.944  45.571  1.00 11.62    A   O
ATOM   54 C   ASP A  7    21.353  66.350  48.670  1.00 10.34    A   C
ATOM   55 O   ASP A  7    20.714  66.410  49.716  1.00 12.06    A   O
ATOM   56 N   SER A  8    21.245  67.262  47.713  1.00 12.07    A   N
ATOM   57 CA  SER A  8    20.330  68.387  47.856  1.00 12.93    A   C
ATOM   58 CB  SER A  8    20.595  69.417  46.756  1.00 12.10    A   C
ATOM   59 OG  SER A  8    20.364  68.857  45.474  1.00 10.24    A   O
ATOM   60 C   SER A  8    18.874  67.909  47.783  1.00 13.34    A   C
ATOM   61 O   SER A  8    17.957  68.609  48.217  1.00 14.16    A   O
ATOM   62 N   GLY A  9    18.667  66.709  47.250  1.00 13.06    A   N
ATOM   63 CA  GLY A  9    17.319  66.182  47.143  1.00 12.56    A   C
ATOM   64 C   GLY A  9    17.253  64.728  46.721  1.00 13.45    A   C
ATOM   65 O   GLY A  9    17.886  63.861  47.329  1.00 13.56    A   O
ATOM   66 N   VAL A 10    16.484  64.460  45.671  1.00 12.87    A   N
ATOM   67 CA  VAL A 10    16.323  63.104  45.159  1.00 12.62    A   C
ATOM   68 CB  VAL A 10    14.916  62.935  44.552  1.00 12.47    A   C
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Figure 7C

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ATOM     69  CG1 VAL A  10      14.715  63.955  43.453  1.00 11.29      A   C
ATOM     70  CG2 VAL A  10      14.720  61.521  44.031  1.00 12.71      A   C
ATOM     71  C   VAL A  10      17.372  62.785  44.095  1.00 12.55      A   C
ATOM     72  O   VAL A  10      17.586  61.624  43.749  1.00 11.19      A   O
ATOM     73  N   GLY A  11      18.020  63.823  43.575  1.00 12.78      A   N
ATOM     74  CA  GLY A  11      19.032  63.623  42.548  1.00 10.57      A   C
ATOM     75  C   GLY A  11      20.039  62.536  42.884  1.00 12.63      A   C
ATOM     76  O   GLY A  11      20.376  61.696  42.035  1.00 12.33      A   O
ATOM     77  N   GLY A  12      20.514  62.560  44.126  1.00 12.27      A   N
ATOM     78  CA  GLY A  12      21.488  61.589  44.597  1.00 13.34      A   C
ATOM     79  C   GLY A  12      21.125  60.142  44.331  1.00 12.55      A   C
ATOM     80  O   GLY A  12      21.963  59.252  44.496  1.00 12.07      A   O
ATOM     81  N   PHE A  13      19.877  59.894  43.938  1.00 11.81      A   N
ATOM     82  CA  PHE A  13      19.447  58.534  43.619  1.00 12.39      A   C
ATOM     83  CB  PHE A  13      18.009  58.515  43.081  1.00 13.67      A   C
ATOM     84  CG  PHE A  13      16.947  58.401  44.148  1.00 13.33      A   C
ATOM     85  CD1 PHE A  13      15.671  57.955  43.816  1.00 14.75      A   C
ATOM     86  CD2 PHE A  13      17.215  58.740  45.470  1.00 13.91      A   C
ATOM     87  CE1 PHE A  13      14.667  57.846  44.790  1.00 18.10      A   C
ATOM     88  CE2 PHE A  13      16.221  58.635  46.454  1.00 15.28      A   C
ATOM     89  CZ  PHE A  13      14.943  58.186  46.112  1.00 13.91      A   C
ATOM     90  C   PHE A  13      20.361  57.940  42.547  1.00 13.92      A   C
ATOM     91  O   PHE A  13      20.630  56.737  42.551  1.00 12.12      A   O
ATOM     92  N   SER A  14      20.827  58.781  41.625  1.00 13.26      A   N
ATOM     93  CA  SER A  14      21.690  58.304  40.547  1.00 13.42      A   C
ATOM     94  CB  SER A  14      21.967  59.423  39.525  1.00 13.96      A   C
ATOM     95  OG  SER A  14      22.695  60.504  40.071  1.00 12.20      A   O
ATOM     96  C   SER A  14      22.992  57.730  41.092  1.00 13.28      A   C
ATOM     97  O   SER A  14      23.559  56.805  40.509  1.00 14.54      A   O
ATOM     98  N   VAL A  15      23.458  58.270  42.214  1.00 10.88      A   N
ATOM     99  CA  VAL A  15      24.674  57.777  42.846  1.00 11.83      A   C
ATOM    100  CB  VAL A  15      25.338  58.859  43.730  1.00 11.43      A   C
ATOM    101  CG1 VAL A  15      26.452  58.243  44.580  1.00 10.44      A   C
ATOM    102  CG2 VAL A  15      25.909  59.960  42.849  1.00 11.65      A   C
ATOM    103  C   VAL A  15      24.333  56.566  43.709  1.00 13.82      A   C
ATOM    104  O   VAL A  15      25.068  55.579  43.727  1.00 13.72      A   O
ATOM    105  N   LEU A  16      23.199  56.635  44.400  1.00 13.39      A   N
ATOM    106  CA  LEU A  16      22.767  55.546  45.264  1.00 14.00      A   C
ATOM    107  CB  LEU A  16      21.479  55.937  45.993  1.00 11.47      A   C
ATOM    108  CG  LEU A  16      20.947  54.898  46.991  1.00 14.59      A   C
ATOM    109  CD1 LEU A  16      22.049  54.511  47.980  1.00 13.56      A   C
ATOM    110  CD2 LEU A  16      19.743  55.477  47.733  1.00 10.24      A   C
ATOM    111  C   LEU A  16      22.562  54.246  44.486  1.00 14.34      A   C
ATOM    112  O   LEU A  16      22.879  53.162  44.980  1.00 13.30      A   O
ATOM    113  N   LYS A  17      22.044  54.356  43.267  1.00 14.05      A   N
ATOM    114  CA  LYS A  17      21.822  53.176  42.438  1.00 16.52      A   C
ATOM    115  CB  LYS A  17      21.229  53.584  41.087  1.00 16.99      A   C
ATOM    116  CG  LYS A  17      21.051  52.424  40.114  1.00 21.73      A   C
ATOM    117  CD  LYS A  17      20.461  52.893  38.802  1.00 24.05      A   C
ATOM    118  CE  LYS A  17      20.298  51.729  37.833  1.00 27.52      A   C
ATOM    119  NZ  LYS A  17      19.805  52.178  36.505  1.00 24.97      A   N
ATOM    120  C   LYS A  17      23.136  52.423  42.220  1.00 17.90      A   C
ATOM    121  O   LYS A  17      23.194  51.193  42.319  1.00 16.07      A   O
ATOM    122  N   SER A  18      24.193  53.171  41.931  1.00 16.04      A   N
ATOM    123  CA  SER A  18      25.508  52.582  41.691  1.00 17.22      A   C
ATOM    124  CB  SER A  18      26.494  53.663  41.248  1.00 16.33      A   C
ATOM    125  OG  SER A  18      26.080  54.255  40.034  1.00 15.13      A   O
ATOM    126  C   SER A  18      26.033  51.900  42.944  1.00 16.33      A   C
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Figure 7D

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ATOM   127  O   SER A  18      26.579  50.795  42.885  1.00 14.32      A   O
ATOM   128  N   LEU A  19      25.863  52.577  44.075  1.00 13.38      A   N
ATOM   129  CA  LEU A  19      26.301  52.072  45.367  1.00 14.03      A   C
ATOM   130  CB  LEU A  19      26.009  53.102  46.456  1.00 11.70      A   C
ATOM   131  CG  LEU A  19      26.748  54.435  46.350  1.00 12.66      A   C
ATOM   132  CD1 LEU A  19      26.284  55.365  47.471  1.00 13.24      A   C
ATOM   133  CD2 LEU A  19      28.248  54.185  46.442  1.00 11.34      A   C
ATOM   134  C   LEU A  19      25.605  50.771  45.720  1.00 15.80      A   C
ATOM   135  O   LEU A  19      26.240  49.831  46.195  1.00 14.57      A   O
ATOM   136  N   LEU A  20      24.294  50.727  45.496  1.00 15.82      A   N
ATOM   137  CA  LEU A  20      23.510  49.540  45.793  1.00 18.19      A   C
ATOM   138  CB  LEU A  20      22.026  49.807  45.515  1.00 16.40      A   C
ATOM   139  CG  LEU A  20      21.346  50.798  46.473  1.00 16.62      A   C
ATOM   140  CD1 LEU A  20      19.949  51.156  45.974  1.00 16.53      A   C
ATOM   141  CD2 LEU A  20      21.279  50.176  47.867  1.00 16.65      A   C
ATOM   142  C   LEU A  20      23.983  48.330  44.988  1.00 20.92      A   C
ATOM   143  O   LEU A  20      24.179  47.247  45.538  1.00 20.94      A   O
ATOM   144  N   LYS A  21      24.169  48.511  43.687  1.00 20.60      A   N
ATOM   145  CA  LYS A  21      24.612  47.406  42.847  1.00 22.68      A   C
ATOM   146  CB  LYS A  21      24.656  47.840  41.380  1.00 21.65      A   C
ATOM   147  CG  LYS A  21      24.973  46.699  40.426  1.00 26.15      A   C
ATOM   148  CD  LYS A  21      25.083  47.169  38.988  1.00 29.67      A   C
ATOM   149  CE  LYS A  21      25.506  46.017  38.078  1.00 34.31      A   C
ATOM   150  NZ  LYS A  21      25.776  46.469  36.684  1.00 32.80      A   N
ATOM   151  C   LYS A  21      25.978  46.863  43.263  1.00 21.58      A   C
ATOM   152  O   LYS A  21      26.214  45.654  43.208  1.00 23.12      A   O
ATOM   153  N   ALA A  22      26.868  47.753  43.692  1.00 19.68      A   N
ATOM   154  CA  ALA A  22      28.216  47.360  44.093  1.00 19.96      A   C
ATOM   155  CB  ALA A  22      29.131  48.585  44.080  1.00 14.81      A   C
ATOM   156  C   ALA A  22      28.317  46.635  45.446  1.00 20.35      A   C
ATOM   157  O   ALA A  22      29.402  46.199  45.839  1.00 21.92      A   O
ATOM   158  N   ARG A  23      27.198  46.509  46.154  1.00 20.50      A   N
ATOM   159  CA  ARG A  23      27.187  45.821  47.444  1.00 21.19      A   C
ATOM   160  CB  ARG A  23      27.205  44.307  47.230  1.00 23.64      A   C
ATOM   161  CG  ARG A  23      25.965  43.756  46.553  1.00 24.47      A   C
ATOM   162  CD  ARG A  23      26.093  42.252  46.372  1.00 30.28      A   C
ATOM   163  NE  ARG A  23      26.418  41.582  47.630  1.00 30.56      A   N
ATOM   164  CZ  ARG A  23      26.768  40.302  47.727  1.00 32.70      A   C
ATOM   165  NH1 ARG A  23      26.838  39.549  46.636  1.00 32.50      A   N
ATOM   166  NH2 ARG A  23      27.054  39.776  48.914  1.00 28.66      A   N
ATOM   167  C   ARG A  23      28.379  46.216  48.302  1.00 21.73      A   C
ATOM   168  O   ARG A  23      29.149  45.365  48.759  1.00 20.27      A   O
ATOM   169  N   LEU A  24      28.522  47.512  48.527  1.00 17.52      A   N
ATOM   170  CA  LEU A  24      29.624  48.018  49.317  1.00 21.03      A   C
ATOM   171  CB  LEU A  24      30.080  49.366  48.757  1.00 20.25      A   C
ATOM   172  CG  LEU A  24      30.478  49.366  47.282  1.00 22.97      A   C
ATOM   173  CD1 LEU A  24      30.723  50.797  46.810  1.00 22.12      A   C
ATOM   174  CD2 LEU A  24      31.723  48.510  47.094  1.00 21.35      A   C
ATOM   175  C   LEU A  24      29.239  48.184  50.776  1.00 21.90      A   C
ATOM   176  O   LEU A  24      30.079  48.032  51.663  1.00 23.97      A   O
ATOM   177  N   PHE A  25      27.968  48.483  51.028  1.00 20.73      A   N
ATOM   178  CA  PHE A  25      27.517  48.710  52.396  1.00 21.16      A   C
ATOM   179  CB  PHE A  25      27.290  50.207  52.609  1.00 19.75      A   C
ATOM   180  CG  PHE A  25      28.416  51.062  52.101  1.00 19.70      A   C
ATOM   181  CD1 PHE A  25      28.249  51.854  50.967  1.00 20.65      A   C
ATOM   182  CD2 PHE A  25      29.648  51.065  52.748  1.00 19.59      A   C
ATOM   183  CE1 PHE A  25      29.294  52.641  50.483  1.00 20.02      A   C
ATOM   184  CE2 PHE A  25      30.701  51.846  52.276  1.00 20.92      A   C
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Figure 7E

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ATOM   185 CZ  PHE A 25     30.522  52.639  51.137  1.00 19.72    A   C
ATOM   186 C   PHE A 25     26.259  47.940  52.773  1.00 18.19    A   C
ATOM   187 O   PHE A 25     25.387  47.718  51.945  1.00 20.08    A   O
ATOM   188 N   ASP A 26     26.174  47.562  54.044  1.00 19.15    A   N
ATOM   189 CA  ASP A 26     25.049  46.793  54.569  1.00 19.40    A   C
ATOM   190 CB  ASP A 26     25.524  45.978  55.768  1.00 21.39    A   C
ATOM   191 CG  ASP A 26     26.764  45.166  55.455  1.00 23.64    A   C
ATOM   192 OD1 ASP A 26     26.632  44.118  54.794  1.00 23.32    A   O
ATOM   193 OD2 ASP A 26     27.875  45.587  55.852  1.00 28.55    A   O
ATOM   194 C   ASP A 26     23.864  47.662  54.978  1.00 18.82    A   C
ATOM   195 O   ASP A 26     22.727  47.196  55.034  1.00 19.35    A   O
ATOM   196 N   GLU A 27     24.132  48.926  55.273  1.00 17.90    A   N
ATOM   197 CA  GLU A 27     23.067  49.840  55.671  1.00 17.07    A   C
ATOM   198 CB  GLU A 27     22.892  49.826  57.187  1.00 17.71    A   C
ATOM   199 CG  GLU A 27     21.646  50.550  57.663  1.00 24.75    A   C
ATOM   200 CD  GLU A 27     21.322  50.279  59.127  1.00 28.18    A   C
ATOM   201 OE1 GLU A 27     20.326  50.846  59.620  1.00 31.23    A   O
ATOM   202 OE2 GLU A 27     22.054  49.500  59.782  1.00 27.47    A   O
ATOM   203 C   GLU A 27     23.393  51.246  55.197  1.00 16.15    A   C
ATOM   204 O   GLU A 27     24.524  51.723  55.346  1.00 14.85    A   O
ATOM   205 N   ILE A 28     22.393  51.910  54.633  1.00 14.40    A   N
ATOM   206 CA  ILE A 28     22.577  53.257  54.118  1.00 12.75    A   C
ATOM   207 CB  ILE A 28     22.574  53.257  52.582  1.00 13.36    A   C
ATOM   208 CG2 ILE A 28     22.678  54.689  52.056  1.00  9.46    A   C
ATOM   209 CG1 ILE A 28     23.736  52.409  52.059  1.00 12.29    A   C
ATOM   210 CD1 ILE A 28     23.699  52.211  50.552  1.00 16.70    A   C
ATOM   211 C   ILE A 28     21.477  54.193  54.592  1.00 13.60    A   C
ATOM   212 O   ILE A 28     20.296  53.854  54.545  1.00 13.62    A   O
ATOM   213 N   ILE A 29     21.879  55.367  55.059  1.00 12.74    A   N
ATOM   214 CA  ILE A 29     20.928  56.375  55.507  1.00 14.14    A   C
ATOM   215 CB  ILE A 29     21.293  56.944  56.893  1.00 13.73    A   C
ATOM   216 CG2 ILE A 29     20.241  57.957  57.324  1.00 15.30    A   C
ATOM   217 CG1 ILE A 29     21.398  55.814  57.929  1.00 15.05    A   C
ATOM   218 CD1 ILE A 29     20.107  55.035  58.145  1.00 14.22    A   C
ATOM   219 C   ILE A 29     21.039  57.489  54.472  1.00 14.66    A   C
ATOM   220 O   ILE A 29     22.056  58.183  54.404  1.00 13.06    A   O
ATOM   221 N   TYR A 30     20.007  57.629  53.648  1.00 12.88    A   N
ATOM   222 CA  TYR A 30     19.987  58.649  52.609  1.00 14.23    A   C
ATOM   223 CB  TYR A 30     19.221  58.133  51.389  1.00 12.46    A   C
ATOM   224 CG  TYR A 30     19.221  59.075  50.205  1.00 15.02    A   C
ATOM   225 CD1 TYR A 30     20.155  58.933  49.178  1.00 12.86    A   C
ATOM   226 CE1 TYR A 30     20.171  59.803  48.088  1.00 12.85    A   C
ATOM   227 CD2 TYR A 30     18.298  60.119  50.117  1.00 15.96    A   C
ATOM   228 CE2 TYR A 30     18.304  60.996  49.034  1.00 15.05    A   C
ATOM   229 CZ  TYR A 30     19.243  60.831  48.023  1.00 14.12    A   C
ATOM   230 OH  TYR A 30     19.248  61.681  46.948  1.00 11.65    A   O
ATOM   231 C   TYR A 30     19.293  59.902  53.139  1.00 15.46    A   C
ATOM   232 O   TYR A 30     18.211  59.815  53.725  1.00 14.07    A   O
ATOM   233 N   TYR A 31     19.909  61.062  52.934  1.00 14.03    A   N
ATOM   234 CA  TYR A 31     19.297  62.312  53.370  1.00 14.37    A   C
ATOM   235 CB  TYR A 31     20.007  62.882  54.601  1.00 13.42    A   C
ATOM   236 CG  TYR A 31     19.441  64.216  55.045  1.00 13.73    A   C
ATOM   237 CD1 TYR A 31     18.150  64.307  55.559  1.00 15.42    A   C
ATOM   238 CE1 TYR A 31     17.616  65.532  55.962  1.00 18.80    A   C
ATOM   239 CD2 TYR A 31     20.191  65.389  54.940  1.00 15.22    A   C
ATOM   240 CE2 TYR A 31     19.665  66.625  55.335  1.00 19.27    A   C
ATOM   241 CZ  TYR A 31     18.376  66.686  55.847  1.00 20.56    A   C
ATOM   242 OH  TYR A 31     17.840  67.894  56.250  1.00 21.50    A   O
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Figure 7F

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ATOM   243  C   TYR A 31     19.321  63.355  52.257  1.00 13.94    A   C
ATOM   244  O   TYR A 31     20.383  63.704  51.743  1.00 12.53    A   O
ATOM   245  N   GLY A 32     18.139  63.836  51.876  1.00 14.52    A   N
ATOM   246  CA  GLY A 32     18.052  64.855  50.846  1.00 11.09    A   C
ATOM   247  C   GLY A 32     17.502  66.137  51.445  1.00 14.21    A   C
ATOM   248  O   GLY A 32     16.474  66.105  52.120  1.00 13.16    A   O
ATOM   249  N   ASP A 33     18.178  67.261  51.217  1.00 11.82    A   N
ATOM   250  CA  ASP A 33     17.728  68.550  51.754  1.00 12.90    A   C
ATOM   251  CB  ASP A 33     18.934  69.474  51.926  1.00 11.25    A   C
ATOM   252  CG  ASP A 33     18.576  70.788  52.587  1.00 11.81    A   C
ATOM   253  OD1 ASP A 33     17.562  70.842  53.309  1.00 14.26    A   O
ATOM   254  OD2 ASP A 33     19.326  71.757  52.394  1.00 11.68    A   O
ATOM   255  C   ASP A 33     16.703  69.145  50.783  1.00 13.65    A   C
ATOM   256  O   ASP A 33     16.824  70.285  50.324  1.00 12.95    A   O
ATOM   257  N   SER A 34     15.693  68.333  50.486  1.00 13.72    A   N
ATOM   258  CA  SER A 34     14.630  68.658  49.543  1.00 14.78    A   C
ATOM   259  CB  SER A 34     13.602  67.527  49.539  1.00 13.92    A   C
ATOM   260  OG  SER A 34     14.230  66.294  49.232  1.00 21.22    A   O
ATOM   261  C   SER A 34     13.914  69.980  49.751  1.00 16.62    A   C
ATOM   262  O   SER A 34     13.379  70.554  48.799  1.00 14.31    A   O
ATOM   263  N   ALA A 35     13.889  70.461  50.990  1.00 13.83    A   N
ATOM   264  CA  ALA A 35     13.216  71.717  51.282  1.00 14.72    A   C
ATOM   265  CB  ALA A 35     13.037  71.875  52.790  1.00 12.61    A   C
ATOM   266  C   ALA A 35     13.982  72.908  50.717  1.00 15.06    A   C
ATOM   267  O   ALA A 35     13.417  73.989  50.538  1.00 17.76    A   O
ATOM   268  N   ARG A 36     15.262  72.713  50.420  1.00 15.20    A   N
ATOM   269  CA  ARG A 36     16.076  73.804  49.902  1.00 15.09    A   C
ATOM   270  CB  ARG A 36     17.175  74.128  50.918  1.00 14.65    A   C
ATOM   271  CG  ARG A 36     16.585  74.462  52.284  1.00 13.95    A   C
ATOM   272  CD  ARG A 36     17.602  75.018  53.255  1.00 15.98    A   C
ATOM   273  NE  ARG A 36     18.579  74.020  53.681  1.00 14.55    A   N
ATOM   274  CZ  ARG A 36     19.333  74.141  54.769  1.00 19.35    A   C
ATOM   275  NH1 ARG A 36     19.217  75.221  55.537  1.00 16.64    A   N
ATOM   276  NH2 ARG A 36     20.201  73.187  55.093  1.00 16.02    A   N
ATOM   277  C   ARG A 36     16.668  73.578  48.511  1.00 15.81    A   C
ATOM   278  O   ARG A 36     17.422  74.409  48.002  1.00 15.67    A   O
ATOM   279  N   VAL A 37     16.319  72.461  47.888  1.00 15.48    A   N
ATOM   280  CA  VAL A 37     16.821  72.168  46.552  1.00 13.76    A   C
ATOM   281  CB  VAL A 37     16.374  70.746  46.115  1.00 14.93    A   C
ATOM   282  CG1 VAL A 37     14.877  70.727  45.851  1.00 14.99    A   C
ATOM   283  CG2 VAL A 37     17.174  70.280  44.898  1.00 14.00    A   C
ATOM   284  C   VAL A 37     16.246  73.243  45.617  1.00 11.66    A   C
ATOM   285  O   VAL A 37     15.112  73.697  45.805  1.00 11.22    A   O
ATOM   286  N   PRO A 38     17.011  73.662  44.596  1.00 12.05    A   N
ATOM   287  CD  PRO A 38     16.485  74.565  43.553  1.00 12.17    A   C
ATOM   288  CA  PRO A 38     18.356  73.214  44.244  1.00 13.67    A   C
ATOM   289  CB  PRO A 38     18.368  73.384  42.736  1.00 14.66    A   C
ATOM   290  CG  PRO A 38     17.655  74.698  42.588  1.00 12.08    A   C
ATOM   291  C   PRO A 38     19.486  74.000  44.898  1.00 15.15    A   C
ATOM   292  O   PRO A 38     19.297  75.129  45.370  1.00 12.96    A   O
ATOM   293  N   TYR A 39     20.664  73.382  44.900  1.00 11.07    A   N
ATOM   294  CA  TYR A 39     21.885  73.974  45.442  1.00 13.74    A   C
ATOM   295  CB  TYR A 39     22.796  72.893  46.040  1.00 11.65    A   C
ATOM   296  CG  TYR A 39     22.461  72.394  47.428  1.00 12.17    A   C
ATOM   297  CD1 TYR A 39     21.229  72.663  48.031  1.00 13.42    A   C
ATOM   298  CE1 TYR A 39     20.932  72.177  49.312  1.00 12.82    A   C
ATOM   299  CD2 TYR A 39     23.387  71.625  48.137  1.00 14.92    A   C
ATOM   300  CE2 TYR A 39     23.103  71.137  49.406  1.00 15.33    A   C
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Figure 7G

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ATOM   301  CZ  TYR A  39      21.878  71.414  49.992  1.00 13.34      A   C
ATOM   302  OH  TYR A  39      21.624  70.941  51.260  1.00 13.24      A   O
ATOM   303  C   TYR A  39      22.654  74.640  44.300  1.00 11.74      A   C
ATOM   304  O   TYR A  39      23.323  75.652  44.494  1.00 14.92      A   O
ATOM   305  N   GLY A  40      22.551  74.049  43.112  1.00 14.63      A   N
ATOM   306  CA  GLY A  40      23.269  74.529  41.939  1.00 12.47      A   C
ATOM   307  C   GLY A  40      23.196  75.993  41.544  1.00 14.09      A   C
ATOM   308  O   GLY A  40      24.093  76.502  40.871  1.00 12.63      A   O
ATOM   309  N   THR A  41      22.141  76.683  41.952  1.00 13.06      A   N
ATOM   310  CA  THR A  41      22.001  78.086  41.585  1.00 17.35      A   C
ATOM   311  CB  THR A  41      20.552  78.400  41.219  1.00 18.12      A   C
ATOM   312  OG1 THR A  41      19.713  78.078  42.332  1.00 22.00      A   O
ATOM   313  CG2 THR A  41      20.115  77.580  40.009  1.00 22.83      A   C
ATOM   314  C   THR A  41      22.416  79.020  42.712  1.00 16.33      A   C
ATOM   315  O   THR A  41      22.266  80.240  42.600  1.00 17.71      A   O
ATOM   316  N   LYS A  42      22.953  78.460  43.787  1.00 14.75      A   N
ATOM   317  CA  LYS A  42      23.331  79.281  44.922  1.00 13.75      A   C
ATOM   318  CB  LYS A  42      22.653  78.721  46.174  1.00 14.86      A   C
ATOM   319  CG  LYS A  42      21.139  78.899  46.078  1.00 14.53      A   C
ATOM   320  CD  LYS A  42      20.342  77.857  46.842  1.00 14.88      A   C
ATOM   321  CE  LYS A  42      18.898  77.878  46.349  1.00 13.95      A   C
ATOM   322  NZ  LYS A  42      17.995  76.929  47.073  1.00 12.60      A   N
ATOM   323  C   LYS A  42      24.824  79.496  45.119  1.00 16.57      A   C
ATOM   324  O   LYS A  42      25.647  78.943  44.391  1.00 14.82      A   O
ATOM   325  N   ASP A  43      25.157  80.329  46.099  1.00 17.21      A   N
ATOM   326  CA  ASP A  43      26.539  80.689  46.390  1.00 19.06      A   C
ATOM   327  CB  ASP A  43      26.567  82.117  46.932  1.00 20.48      A   C
ATOM   328  CG  ASP A  43      25.808  82.245  48.228  1.00 21.34      A   C
ATOM   329  OD1 ASP A  43      26.458  82.356  49.287  1.00 19.30      A   O
ATOM   330  OD2 ASP A  43      24.557  82.210  48.190  1.00 23.52      A   O
ATOM   331  C   ASP A  43      27.260  79.763  47.371  1.00 19.43      A   C
ATOM   332  O   ASP A  43      26.634  79.034  48.141  1.00 18.30      A   O
ATOM   333  N   PRO A  44      28.604  79.789  47.346  1.00 21.23      A   N
ATOM   334  CD  PRO A  44      29.401  80.567  46.377  1.00 20.65      A   C
ATOM   335  CA  PRO A  44      29.482  78.984  48.202  1.00 20.54      A   C
ATOM   336  CB  PRO A  44      30.866  79.543  47.886  1.00 20.91      A   C
ATOM   337  CG  PRO A  44      30.749  79.881  46.440  1.00 20.03      A   C
ATOM   338  C   PRO A  44      29.165  79.051  49.691  1.00 21.08      A   C
ATOM   339  O   PRO A  44      29.078  78.020  50.362  1.00 22.03      A   O
ATOM   340  N   THR A  45      28.999  80.266  50.207  1.00 20.06      A   N
ATOM   341  CA  THR A  45      28.707  80.453  51.622  1.00 19.83      A   C
ATOM   342  CB  THR A  45      28.523  81.953  51.961  1.00 22.19      A   C
ATOM   343  OG1 THR A  45      29.734  82.659  51.667  1.00 22.93      A   O
ATOM   344  CG2 THR A  45      28.180  82.135  53.429  1.00 21.29      A   C
ATOM   345  C   THR A  45      27.453  79.697  52.027  1.00 18.90      A   C
ATOM   346  O   THR A  45      27.448  78.950  53.007  1.00 16.82      A   O
ATOM   347  N   THR A  46      26.386  79.893  51.263  1.00 17.42      A   N
ATOM   348  CA  THR A  46      25.125  79.235  51.546  1.00 17.81      A   C
ATOM   349  CB  THR A  46      24.039  79.671  50.542  1.00 16.98      A   C
ATOM   350  OG1 THR A  46      23.835  81.087  50.636  1.00 17.53      A   O
ATOM   351  CG2 THR A  46      22.737  78.971  50.839  1.00 19.05      A   C
ATOM   352  C   THR A  46      25.265  77.719  51.484  1.00 17.51      A   C
ATOM   353  O   THR A  46      24.766  77.004  52.355  1.00 18.78      A   O
ATOM   354  N   ILE A  47      25.945  77.236  50.452  1.00 17.91      A   N
ATOM   355  CA  ILE A  47      26.134  75.803  50.265  1.00 20.81      A   C
ATOM   356  CB  ILE A  47      26.822  75.513  48.912  1.00 20.52      A   C
ATOM   357  CG2 ILE A  47      26.934  74.002  48.678  1.00 18.34      A   C
ATOM   358  CG1 ILE A  47      26.004  76.143  47.783  1.00 23.35      A   C
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Figure 7H

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ATOM   359  CD1 ILE A  47      24.523  75.792  47.826  1.00 23.82      A   C
ATOM   360  C   ILE A  47      26.935  75.170  51.398  1.00 19.27      A   C
ATOM   361  O   ILE A  47      26.568  74.111  51.905  1.00 21.96      A   O
ATOM   362  N   LYS A  48      28.018  75.818  51.805  1.00 21.30      A   N
ATOM   363  CA  LYS A  48      28.834  75.292  52.890  1.00 20.85      A   C
ATOM   364  CB  LYS A  48      30.032  76.203  53.151  1.00 22.83      A   C
ATOM   365  CG  LYS A  48      31.094  76.059  52.091  1.00 27.64      A   C
ATOM   366  CD  LYS A  48      32.380  76.794  52.444  1.00 31.38      A   C
ATOM   367  CE  LYS A  48      32.246  78.287  52.245  1.00 32.58      A   C
ATOM   368  NZ  LYS A  48      33.567  78.966  52.404  1.00 35.58      A   N
ATOM   369  C   LYS A  48      28.029  75.101  54.163  1.00 21.38      A   C
ATOM   370  O   LYS A  48      28.141  74.061  54.814  1.00 20.76      A   O
ATOM   371  N   GLN A  49      27.211  76.091  54.520  1.00 19.20      A   N
ATOM   372  CA  GLN A  49      26.395  75.963  55.716  1.00 19.40      A   C
ATOM   373  CB  GLN A  49      25.619  77.256  56.005  1.00 19.30      A   C
ATOM   374  CG  GLN A  49      24.776  77.203  57.286  1.00 22.44      A   C
ATOM   375  CD  GLN A  49      25.581  76.812  58.525  1.00 20.73      A   C
ATOM   376  OE1 GLN A  49      26.740  77.192  58.667  1.00 22.79      A   O
ATOM   377  NE2 GLN A  49      24.958  76.068  59.433  1.00 22.60      A   N
ATOM   378  C   GLN A  49      25.423  74.803  55.553  1.00 18.14      A   C
ATOM   379  O   GLN A  49      25.159  74.074  56.510  1.00 19.87      A   O
ATOM   380  N   PHE A  50      24.882  74.631  54.348  1.00 17.65      A   N
ATOM   381  CA  PHE A  50      23.960  73.521  54.112  1.00 17.56      A   C
ATOM   382  CB  PHE A  50      23.461  73.510  52.659  1.00 17.20      A   C
ATOM   383  CG  PHE A  50      22.478  74.604  52.331  1.00 18.53      A   C
ATOM   384  CD1 PHE A  50      21.961  75.433  53.323  1.00 18.95      A   C
ATOM   385  CD2 PHE A  50      22.041  74.780  51.022  1.00 20.21      A   C
ATOM   386  CE1 PHE A  50      21.023  76.418  53.022  1.00 19.32      A   C
ATOM   387  CE2 PHE A  50      21.101  75.763  50.709  1.00 22.48      A   C
ATOM   388  CZ  PHE A  50      20.592  76.583  51.716  1.00 21.15      A   C
ATOM   389  C   PHE A  50      24.706  72.217  54.401  1.00 15.70      A   C
ATOM   390  O   PHE A  50      24.178  71.311  55.048  1.00 15.38      A   O
ATOM   391  N   GLY A  51      25.945  72.143  53.922  1.00 18.19      A   N
ATOM   392  CA  GLY A  51      26.760  70.959  54.126  1.00 19.41      A   C
ATOM   393  C   GLY A  51      27.006  70.667  55.592  1.00 20.96      A   C
ATOM   394  O   GLY A  51      26.964  69.514  56.026  1.00 20.04      A   O
ATOM   395  N   LEU A  52      27.261  71.716  56.368  1.00 22.33      A   N
ATOM   396  CA  LEU A  52      27.508  71.542  57.791  1.00 22.23      A   C
ATOM   397  CB  LEU A  52      27.995  72.855  58.412  1.00 24.46      A   C
ATOM   398  CG  LEU A  52      29.385  73.328  57.980  1.00 25.92      A   C
ATOM   399  CD1 LEU A  52      29.734  74.618  58.719  1.00 28.98      A   C
ATOM   400  CD2 LEU A  52      30.423  72.249  58.293  1.00 27.40      A   C
ATOM   401  C   LEU A  52      26.246  71.063  58.493  1.00 21.84      A   C
ATOM   402  O   LEU A  52      26.294  70.180  59.344  1.00 21.12      A   O
ATOM   403  N   GLU A  53      25.107  71.635  58.124  1.00 20.72      A   N
ATOM   404  CA  GLU A  53      23.852  71.237  58.736  1.00 20.40      A   C
ATOM   405  CB  GLU A  53      22.731  72.185  58.294  1.00 21.74      A   C
ATOM   406  CG  GLU A  53      22.655  73.438  59.159  1.00 21.95      A   C
ATOM   407  CD  GLU A  53      21.839  74.551  58.536  1.00 23.86      A   C
ATOM   408  OE1 GLU A  53      20.797  74.260  57.906  1.00 23.19      A   O
ATOM   409  OE2 GLU A  53      22.238  75.727  58.685  1.00 24.44      A   O
ATOM   410  C   GLU A  53      23.514  69.789  58.405  1.00 19.46      A   C
ATOM   411  O   GLU A  53      22.813  69.122  59.160  1.00 22.12      A   O
ATOM   412  N   ALA A  54      24.022  69.295  57.282  1.00 20.85      A   N
ATOM   413  CA  ALA A  54      23.760  67.910  56.905  1.00 18.16      A   C
ATOM   414  CB  ALA A  54      24.252  67.647  55.498  1.00 16.88      A   C
ATOM   415  C   ALA A  54      24.474  66.997  57.899  1.00 18.85      A   C
ATOM   416  O   ALA A  54      23.953  65.944  58.280  1.00 18.10      A   O
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Figure 7I

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ATOM   417 N   LEU A 55    25.670 67.408 58.313 1.00 19.45    A   N
ATOM   418 CA  LEU A 55    26.442 66.639 59.281 1.00 19.66    A   C
ATOM   419 CB  LEU A 55    27.775 67.329 59.590 1.00 21.26    A   C
ATOM   420 CG  LEU A 55    28.782 67.408 58.442 1.00 22.31    A   C
ATOM   421 CD1 LEU A 55    30.070 68.042 58.935 1.00 21.17    A   C
ATOM   422 CD2 LEU A 55    29.055 66.008 57.898 1.00 22.77    A   C
ATOM   423 C   LEU A 55    25.626 66.504 60.556 1.00 21.84    A   C
ATOM   424 O   LEU A 55    25.589 65.437 61.166 1.00 20.58    A   O
ATOM   425 N   ASP A 56    24.959 67.584 60.953 1.00 21.85    A   N
ATOM   426 CA  ASP A 56    24.147 67.543 62.157 1.00 22.53    A   C
ATOM   427 CB  ASP A 56    23.506 68.904 62.437 1.00 25.87    A   C
ATOM   428 CG  ASP A 56    24.530 69.986 62.715 1.00 29.28    A   C
ATOM   429 OD1 ASP A 56    25.636 69.651 63.190 1.00 31.33    A   O
ATOM   430 OD2 ASP A 56    24.226 71.172 62.473 1.00 32.07    A   O
ATOM   431 C   ASP A 56    23.062 66.492 62.023 1.00 22.75    A   C
ATOM   432 O   ASP A 56    22.777 65.762 62.974 1.00 22.74    A   O
ATOM   433 N   PHE A 57    22.459 66.403 60.841 1.00 20.21    A   N
ATOM   434 CA  PHE A 57    21.404 65.422 60.633 1.00 21.09    A   C
ATOM   435 CB  PHE A 57    20.831 65.497 59.215 1.00 21.92    A   C
ATOM   436 CG  PHE A 57    19.915 64.352 58.893 1.00 21.43    A   C
ATOM   437 CD1 PHE A 57    18.609 64.336 59.370 1.00 22.87    A   C
ATOM   438 CD2 PHE A 57    20.393 63.233 58.214 1.00 20.64    A   C
ATOM   439 CE1 PHE A 57    17.792 63.218 59.184 1.00 20.01    A   C
ATOM   440 CE2 PHE A 57    19.589 62.112 58.024 1.00 21.14    A   C
ATOM   441 CZ  PHE A 57    18.286 62.104 58.512 1.00 23.52    A   C
ATOM   442 C   PHE A 57    21.873 63.991 60.864 1.00 18.61    A   C
ATOM   443 O   PHE A 57    21.148 63.181 61.441 1.00 20.52    A   O
ATOM   444 N   PHE A 58    23.081 63.679 60.408 1.00 19.51    A   N
ATOM   445 CA  PHE A 58    23.615 62.324 60.532 1.00 21.64    A   C
ATOM   446 CB  PHE A 58    24.701 62.097 59.478 1.00 18.15    A   C
ATOM   447 CG  PHE A 58    24.181 62.018 58.072 1.00 17.07    A   C
ATOM   448 CD1 PHE A 58    24.380 63.072 57.180 1.00 15.61    A   C
ATOM   449 CD2 PHE A 58    23.508 60.878 57.628 1.00 16.58    A   C
ATOM   450 CE1 PHE A 58    23.920 62.993 55.868 1.00 16.17    A   C
ATOM   451 CE2 PHE A 58    23.044 60.790 56.318 1.00 20.24    A   C
ATOM   452 CZ  PHE A 58    23.251 61.850 55.436 1.00 14.25    A   C
ATOM   453 C   PHE A 58    24.164 61.894 61.896 1.00 24.25    A   C
ATOM   454 O   PHE A 58    24.323 60.697 62.147 1.00 24.91    A   O
ATOM   455 N   LYS A 59    24.449 62.850 62.774 1.00 26.87    A   N
ATOM   456 CA  LYS A 59    25.014 62.528 64.087 1.00 28.83    A   C
ATOM   457 CB  LYS A 59    25.116 63.800 64.931 1.00 31.02    A   C
ATOM   458 CG  LYS A 59    26.127 64.792 64.374 1.00 33.56    A   C
ATOM   459 CD  LYS A 59    26.237 66.047 65.221 1.00 37.86    A   C
ATOM   460 CE  LYS A 59    27.270 67.000 64.632 1.00 38.94    A   C
ATOM   461 NZ  LYS A 59    27.433 68.240 65.443 1.00 41.75    A   N
ATOM   462 C   LYS A 59    24.312 61.419 64.879 1.00 28.21    A   C
ATOM   463 O   LYS A 59    24.973 60.541 65.439 1.00 28.12    A   O
ATOM   464 N   PRO A 60    22.969 61.437 64.933 1.00 27.85    A   N
ATOM   465 CD  PRO A 60    22.061 62.472 64.412 1.00 27.44    A   C
ATOM   466 CA  PRO A 60    22.219 60.409 65.671 1.00 26.21    A   C
ATOM   467 CB  PRO A 60    20.791 60.962 65.691 1.00 28.29    A   C
ATOM   468 CG  PRO A 60    20.961 62.446 65.419 1.00 29.74    A   C
ATOM   469 C   PRO A 60    22.264 59.040 64.994 1.00 25.09    A   C
ATOM   470 O   PRO A 60    22.116 58.004 65.640 1.00 24.61    A   O
ATOM   471 N   HIS A 61    22.469 59.045 63.682 1.00 24.30    A   N
ATOM   472 CA  HIS A 61    22.489 57.815 62.906 1.00 23.28    A   C
ATOM   473 CB  HIS A 61    22.210 58.148 61.445 1.00 23.75    A   C
ATOM   474 CG  HIS A 61    20.813 58.616 61.202 1.00 23.81    A   C
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Figure 7J

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ATOM   475  CD2 HIS A  61      20.307  59.858  61.017  1.00 24.28      A   C
ATOM   476  ND1 HIS A  61      19.738  57.753  61.163  1.00 21.57      A   N
ATOM   477  CE1 HIS A  61      18.631  58.443  60.963  1.00 21.88      A   C
ATOM   478  NE2 HIS A  61      18.948  59.723  60.871  1.00 24.37      A   N
ATOM   479  C   HIS A  61     23.754  56.979  63.012  1.00 23.45      A   C
ATOM   480  O   HIS A  61     23.812  55.879  62.475  1.00 23.17      A   O
ATOM   481  N   GLU A  62      24.752  57.497  63.718  1.00 26.52      A   N
ATOM   482  CA  GLU A  62      26.030  56.811  63.892  1.00 27.77      A   C
ATOM   483  CB  GLU A  62      25.944  55.818  65.062  1.00 33.97      A   C
ATOM   484  CG  GLU A  62      24.861  54.754  64.943  1.00 37.16      A   C
ATOM   485  CD  GLU A  62      24.468  54.176  66.292  1.00 40.46      A   C
ATOM   486  OE1 GLU A  62      25.367  53.907  67.117  1.00 41.12      A   O
ATOM   487  OE2 GLU A  62      23.255  53.983  66.525  1.00 42.43      A   O
ATOM   488  C   GLU A  62      26.545  56.118  62.626  1.00 26.21      A   C
ATOM   489  O   GLU A  62      26.699  54.897  62.579  1.00 26.16      A   O
ATOM   490  N   ILE A  63     26.798  56.913  61.591  1.00 22.24      A   N
ATOM   491  CA  ILE A  63      27.333  56.385  60.338  1.00 21.10      A   C
ATOM   492  CB  ILE A  63      26.904  57.246  59.124  1.00 19.78      A   C
ATOM   493  CG2 ILE A  63      25.416  57.065  58.859  1.00 15.78      A   C
ATOM   494  CG1 ILE A  63      27.224  58.718  59.388  1.00 16.88      A   C
ATOM   495  CD1 ILE A  63      27.000  59.636  58.189  1.00 18.48      A   C
ATOM   496  C   ILE A  63     28.853  56.420  60.483  1.00 18.95      A   C
ATOM   497  O   ILE A  63     29.385  57.182  61.293  1.00 19.85      A   O
ATOM   498  N   GLU A  64      29.553  55.593  59.718  1.00 19.95      A   N
ATOM   499  CA  GLU A  64      31.008  55.561  59.804  1.00 19.49      A   C
ATOM   500  CB  GLU A  64      31.492  54.118  59.926  1.00 22.43      A   C
ATOM   501  CG  GLU A  64      31.139  53.498  61.268  1.00 26.80      A   C
ATOM   502  CD  GLU A  64      31.762  52.136  61.452  1.00 29.61      A   C
ATOM   503  OE1 GLU A  64      33.012  52.044  61.421  1.00 31.41      A   O
ATOM   504  OE2 GLU A  64      31.003  51.160  61.623  1.00 29.53      A   O
ATOM   505  C   GLU A  64      31.684  56.251  58.630  1.00 17.37      A   C
ATOM   506  O   GLU A  64      32.890  56.453  58.631  1.00 16.28      A   O
ATOM   507  N   LEU A  65      30.890  56.615  57.632  1.00 18.28      A   N
ATOM   508  CA  LEU A  65      31.393  57.308  56.456  1.00 17.15      A   C
ATOM   509  CB  LEU A  65      32.035  56.318  55.478  1.00 18.66      A   C
ATOM   510  CG  LEU A  65      32.582  56.903  54.169  1.00 21.47      A   C
ATOM   511  CD1 LEU A  65      33.667  55.991  53.603  1.00 23.00      A   C
ATOM   512  CD2 LEU A  65      31.449  57.086  53.167  1.00 22.69      A   C
ATOM   513  C   LEU A  65     30.230  58.021  55.786  1.00 16.52      A   C
ATOM   514  O   LEU A  65      29.100  57.539  55.813  1.00 14.91      A   O
ATOM   515  N   LEU A  66      30.510  59.180  55.204  1.00 14.90      A   N
ATOM   516  CA  LEU A  66      29.486  59.946  54.526  1.00 14.23      A   C
ATOM   517  CB  LEU A  66      29.264  61.288  55.231  1.00 14.12      A   C
ATOM   518  CG  LEU A  66      28.297  62.240  54.514  1.00 14.20      A   C
ATOM   519  CD1 LEU A  66      26.932  61.586  54.415  1.00 14.73      A   C
ATOM   520  CD2 LEU A  66      28.195  63.562  55.262  1.00 13.86      A   C
ATOM   521  C   LEU A  66     29.864  60.200  53.077  1.00 14.92      A   C
ATOM   522  O   LEU A  66      30.975  60.642  52.773  1.00 14.96      A   O
ATOM   523  N   ILE A  67     28.938  59.886  52.181  1.00 13.46      A   N
ATOM   524  CA  ILE A  67      29.140  60.124  50.766  1.00 12.96      A   C
ATOM   525  CB  ILE A  67      28.641  58.953  49.886  1.00 13.86      A   C
ATOM   526  CG2 ILE A  67      28.617  59.385  48.419  1.00 12.97      A   C
ATOM   527  CG1 ILE A  67      29.541  57.729  50.066  1.00 14.37      A   C
ATOM   528  CD1 ILE A  67      29.105  56.530  49.237  1.00 18.27      A   C
ATOM   529  C   ILE A  67     28.314  61.346  50.406  1.00 12.36      A   C
ATOM   530  O   ILE A  67      27.116  61.420  50.719  1.00 13.82      A   O
ATOM   531  N   VAL A  68      28.964  62.317  49.780  1.00 12.37      A   N
ATOM   532  CA  VAL A  68      28.275  63.516  49.342  1.00 12.34      A   C
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Figure 7K

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ATOM   533 CB  VAL A 68     29.160  64.759  49.466  1.00 10.71    A   C
ATOM   534 CG1 VAL A 68     28.413  65.977  48.916  1.00 10.16    A   C
ATOM   535 CG2 VAL A 68     29.525  64.978  50.927  1.00 11.52    A   C
ATOM   536 C   VAL A 68     28.002  63.222  47.884  1.00 11.20    A   C
ATOM   537 O   VAL A 68     28.885  63.362  47.038  1.00 12.44    A   O
ATOM   538 N   ALA A 69     26.785  62.775  47.602  1.00  9.18    A   N
ATOM   539 CA  ALA A 69     26.405  62.415  46.244  1.00 10.89    A   C
ATOM   540 CB  ALA A 69     25.129  61.581  46.263  1.00  9.29    A   C
ATOM   541 C   ALA A 69     26.218  63.631  45.358  1.00 10.34    A   C
ATOM   542 O   ALA A 69     26.341  63.546  44.139  1.00 11.20    A   O
ATOM   543 N   CYS A 70     25.905  64.760  45.982  1.00 10.65    A   N
ATOM   544 CA  CYS A 70     25.692  66.000  45.253  1.00 11.99    A   C
ATOM   545 CB  CYS A 70     25.026  67.030  46.167  1.00 13.56    A   C
ATOM   546 SG  CYS A 70     24.697  68.605  45.370  1.00 10.79    A   S
ATOM   547 C   CYS A 70     27.004  66.560  44.720  1.00 11.25    A   C
ATOM   548 O   CYS A 70     27.981  66.708  45.463  1.00  9.23    A   O
ATOM   549 N   ASN A 71     27.030  66.867  43.425  1.00 10.81    A   N
ATOM   550 CA  ASN A 71     28.228  67.424  42.807  1.00  9.85    A   C
ATOM   551 CB  ASN A 71     28.120  67.369  41.285  1.00  7.25    A   C
ATOM   552 CG  ASN A 71     28.026  65.959  40.768  1.00  9.24    A   C
ATOM   553 OD1 ASN A 71     26.998  65.298  40.919  1.00  8.82    A   O
ATOM   554 ND2 ASN A 71     29.107  65.478  40.165  1.00  9.13    A   N
ATOM   555 C   ASN A 71     28.434  68.866  43.246  1.00 12.09    A   C
ATOM   556 O   ASN A 71     29.565  69.321  43.432  1.00  9.50    A   O
ATOM   557 N   THR A 72     27.337  69.593  43.399  1.00 10.94    A   N
ATOM   558 CA  THR A 72     27.436  70.975  43.834  1.00 10.39    A   C
ATOM   559 CB  THR A 72     26.073  71.676  43.779  1.00  9.07    A   C
ATOM   560 OG1 THR A 72     25.599  71.675  42.429  1.00 10.15    A   O
ATOM   561 CG2 THR A 72     26.200  73.122  44.262  1.00  9.53    A   C
ATOM   562 C   THR A 72     27.974  71.029  45.259  1.00 11.47    A   C
ATOM   563 O   THR A 72     28.882  71.808  45.556  1.00  9.49    A   O
ATOM   564 N   ALA A 73     27.415  70.202  46.144  1.00 13.67    A   N
ATOM   565 CA  ALA A 73     27.871  70.171  47.531  1.00 13.27    A   C
ATOM   566 CB  ALA A 73     26.979  69.251  48.368  1.00 15.12    A   C
ATOM   567 C   ALA A 73     29.318  69.691  47.586  1.00 15.74    A   C
ATOM   568 O   ALA A 73     30.111  70.160  48.412  1.00 15.99    A   O
ATOM   569 N   SER A 74     29.660  68.746  46.714  1.00 13.48    A   N
ATOM   570 CA  SER A 74     31.021  68.226  46.677  1.00 13.55    A   C
ATOM   571 CB  SER A 74     31.133  67.078  45.665  1.00 10.32    A   C
ATOM   572 OG  SER A 74     30.483  65.916  46.148  1.00 14.22    A   O
ATOM   573 C   SER A 74     31.994  69.333  46.297  1.00 15.60    A   C
ATOM   574 O   SER A 74     33.093  69.439  46.845  1.00 14.18    A   O
ATOM   575 N   ALA A 75     31.578  70.169  45.359  1.00 13.93    A   N
ATOM   576 CA  ALA A 75     32.422  71.259  44.899  1.00 15.79    A   C
ATOM   577 CB  ALA A 75     31.899  71.773  43.560  1.00 16.15    A   C
ATOM   578 C   ALA A 75     32.549  72.420  45.886  1.00 17.44    A   C
ATOM   579 O   ALA A 75     33.639  72.967  46.063  1.00 18.83    A   O
ATOM   580 N   LEU A 76     31.453  72.777  46.548  1.00 15.33    A   N
ATOM   581 CA  LEU A 76     31.462  73.920  47.460  1.00 17.71    A   C
ATOM   582 CB  LEU A 76     30.236  74.793  47.189  1.00 16.64    A   C
ATOM   583 CG  LEU A 76     30.154  75.642  45.917  1.00 19.98    A   C
ATOM   584 CD1 LEU A 76     30.338  74.793  44.681  1.00 15.78    A   C
ATOM   585 CD2 LEU A 76     28.801  76.343  45.886  1.00 19.48    A   C
ATOM   586 C   LEU A 76     31.544  73.693  48.967  1.00 18.84    A   C
ATOM   587 O   LEU A 76     32.101  74.531  49.685  1.00 17.49    A   O
ATOM   588 N   ALA A 77     30.996  72.584  49.456  1.00 16.91    A   N
ATOM   589 CA  ALA A 77     30.986  72.338  50.896  1.00 17.45    A   C
ATOM   590 CB  ALA A 77     29.546  72.118  51.363  1.00 15.97    A   C
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Figure 7L

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ATOM   591  C   ALA A  77     31.862  71.206  51.422  1.00 17.05      A   C
ATOM   592  O   ALA A  77     32.092  71.120  52.630  1.00 15.31      A   O
ATOM   593  N   LEU A  78     32.355  70.350  50.533  1.00 17.95      A   N
ATOM   594  CA  LEU A  78     33.173  69.217  50.950  1.00 18.28      A   C
ATOM   595  CB  LEU A  78     33.701  68.456  49.726  1.00 17.49      A   C
ATOM   596  CG  LEU A  78     34.425  67.141  50.053  1.00 18.47      A   C
ATOM   597  CD1 LEU A  78     33.467  66.196  50.771  1.00 13.07      A   C
ATOM   598  CD2 LEU A  78     34.949  66.493  48.772  1.00 15.57      A   C
ATOM   599  C   LEU A  78     34.337  69.572  51.873  1.00 19.44      A   C
ATOM   600  O   LEU A  78     34.478  68.986  52.944  1.00 17.85      A   O
ATOM   601  N   GLU A  79     35.173  70.524  51.472  1.00 20.74      A   N
ATOM   602  CA  GLU A  79     36.310  70.897  52.304  1.00 23.29      A   C
ATOM   603  CB  GLU A  79     37.112  72.023  51.652  1.00 25.50      A   C
ATOM   604  CG  GLU A  79     38.332  72.435  52.464  1.00 32.40      A   C
ATOM   605  CD  GLU A  79     39.248  73.382  51.714  1.00 36.37      A   C
ATOM   606  OE1 GLU A  79     38.811  74.501  51.377  1.00 38.33      A   O
ATOM   607  OE2 GLU A  79     40.411  73.002  51.459  1.00 40.30      A   O
ATOM   608  C   GLU A  79     35.900  71.312  53.716  1.00 22.08      A   C
ATOM   609  O   GLU A  79     36.512  70.888  54.691  1.00 22.83      A   O
ATOM   610  N   GLU A  80     34.862  72.132  53.825  1.00 22.05      A   N
ATOM   611  CA  GLU A  80     34.399  72.591  55.125  1.00 21.68      A   C
ATOM   612  CB  GLU A  80     33.336  73.675  54.957  1.00 26.13      A   C
ATOM   613  CG  GLU A  80     33.081  74.457  56.232  1.00 32.22      A   C
ATOM   614  CD  GLU A  80     34.173  75.479  56.521  1.00 34.38      A   C
ATOM   615  OE1 GLU A  80     35.371  75.145  56.399  1.00 36.64      A   O
ATOM   616  OE2 GLU A  80     33.828  76.623  56.878  1.00 38.94      A   O
ATOM   617  C   GLU A  80     33.823  71.435  55.939  1.00 21.19      A   C
ATOM   618  O   GLU A  80     34.013  71.359  57.152  1.00 20.49      A   O
ATOM   619  N   MET A  81     33.116  70.533  55.269  1.00 18.90      A   N
ATOM   620  CA  MET A  81     32.531  69.389  55.950  1.00 16.84      A   C
ATOM   621  CB  MET A  81     31.639  68.605  54.992  1.00 14.00      A   C
ATOM   622  CG  MET A  81     30.375  69.349  54.615  1.00 15.86      A   C
ATOM   623  SD  MET A  81     29.517  68.583  53.244  1.00 15.74      A   S
ATOM   624  CE  MET A  81     28.866  67.134  54.019  1.00 14.04      A   C
ATOM   625  C   MET A  81     33.618  68.474  56.503  1.00 17.31      A   C
ATOM   626  O   MET A  81     33.539  68.020  57.646  1.00 16.49      A   O
ATOM   627  N   GLN A  82     34.632  68.216  55.684  1.00 18.90      A   N
ATOM   628  CA  GLN A  82     35.739  67.351  56.078  1.00 22.12      A   C
ATOM   629  CB  GLN A  82     36.674  67.125  54.887  1.00 22.92      A   C
ATOM   630  CG  GLN A  82     36.001  66.442  53.706  1.00 21.03      A   C
ATOM   631  CD  GLN A  82     36.961  66.158  52.575  1.00 22.15      A   C
ATOM   632  OE1 GLN A  82     37.725  67.033  52.159  1.00 22.13      A   O
ATOM   633  NE2 GLN A  82     36.924  64.934  52.061  1.00 20.69      A   N
ATOM   634  C   GLN A  82     36.516  67.956  57.237  1.00 24.53      A   C
ATOM   635  O   GLN A  82     37.051  67.239  58.086  1.00 23.68      A   O
ATOM   636  N   LYS A  83     36.565  69.282  57.271  1.00 26.24      A   N
ATOM   637  CA  LYS A  83     37.282  69.993  58.317  1.00 30.03      A   C
ATOM   638  CB  LYS A  83     37.178  71.505  58.092  1.00 30.40      A   C
ATOM   639  CG  LYS A  83     38.023  72.336  59.041  1.00 34.26      A   C
ATOM   640  CD  LYS A  83     37.873  73.829  58.756  1.00 38.51      A   C
ATOM   641  CE  LYS A  83     38.287  74.175  57.329  1.00 42.25      A   C
ATOM   642  NZ  LYS A  83     38.067  75.619  57.005  1.00 43.57      A   N
ATOM   643  C   LYS A  83     36.764  69.650  59.708  1.00 30.42      A   C
ATOM   644  O   LYS A  83     37.551  69.395  60.616  1.00 31.77      A   O
ATOM   645  N   TYR A  84     35.445  69.624  59.870  1.00 30.72      A   N
ATOM   646  CA  TYR A  84     34.850  69.341  61.173  1.00 34.49      A   C
ATOM   647  CB  TYR A  84     33.702  70.322  61.441  1.00 38.58      A   C
ATOM   648  CG  TYR A  84     34.109  71.781  61.386  1.00 43.85      A   C
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Figure 7M

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ATOM   649 CD1 TYR A 84     34.172  72.465  60.169  1.00 45.26      A   C
ATOM   650 CE1 TYR A 84     34.575  73.803  60.111  1.00 46.74      A   C
ATOM   651 CD2 TYR A 84     34.460  72.472  62.549  1.00 45.80      A   C
ATOM   652 CE2 TYR A 84     34.865  73.808  62.501  1.00 47.25      A   C
ATOM   653 CZ  TYR A 84     34.920  74.467  61.281  1.00 47.45      A   C
ATOM   654 OH  TYR A 84     35.321  75.784  61.233  1.00 47.13      A   O
ATOM   655 C   TYR A 84     34.349  67.911  61.401  1.00 33.43      A   C
ATOM   656 O   TYR A 84     33.973  67.555  62.520  1.00 34.46      A   O
ATOM   657 N   SER A 85     34.348  67.088  60.361  1.00 30.46      A   N
ATOM   658 CA  SER A 85     33.865  65.721  60.507  1.00 27.21      A   C
ATOM   659 CB  SER A 85     33.384  65.192  59.160  1.00 26.99      A   C
ATOM   660 OG  SER A 85     33.003  63.836  59.279  1.00 27.59      A   O
ATOM   661 C   SER A 85     34.883  64.745  61.088  1.00 25.50      A   C
ATOM   662 O   SER A 85     36.059  64.778  60.730  1.00 24.71      A   O
ATOM   663 N   LYS A 86     34.415  63.875  61.981  1.00 23.68      A   N
ATOM   664 CA  LYS A 86     35.265  62.868  62.609  1.00 23.93      A   C
ATOM   665 CB  LYS A 86     34.741  62.509  64.005  1.00 26.65      A   C
ATOM   666 CG  LYS A 86     34.774  63.644  65.028  1.00 31.69      A   C
ATOM   667 CD  LYS A 86     36.190  63.990  65.491  1.00 34.31      A   C
ATOM   668 CE  LYS A 86     37.015  64.657  64.401  1.00 35.72      A   C
ATOM   669 NZ  LYS A 86     38.359  65.087  64.902  1.00 41.28      A   N
ATOM   670 C   LYS A 86     35.308  61.607  61.752  1.00 22.61      A   C
ATOM   671 O   LYS A 86     36.192  60.765  61.914  1.00 23.21      A   O
ATOM   672 N   ILE A 87     34.337  61.462  60.857  1.00 19.67      A   N
ATOM   673 CA  ILE A 87     34.305  60.302  59.975  1.00 18.68      A   C
ATOM   674 CB  ILE A 87     32.896  59.681  59.888  1.00 18.75      A   C
ATOM   675 CG2 ILE A 87     32.510  59.090  61.233  1.00 18.89      A   C
ATOM   676 CG1 ILE A 87     31.887  60.742  59.433  1.00 21.06      A   C
ATOM   677 CD1 ILE A 87     30.508  60.187  59.086  1.00 18.90      A   C
ATOM   678 C   ILE A 87     34.720  60.751  58.585  1.00 16.98      A   C
ATOM   679 O   ILE A 87     34.614  61.932  58.248  1.00 16.62      A   O
ATOM   680 N   PRO A 88     35.219  59.822  57.761  1.00 17.72      A   N
ATOM   681 CD  PRO A 88     35.548  58.403  57.992  1.00 17.09      A   C
ATOM   682 CA  PRO A 88     35.616  60.247  56.418  1.00 17.99      A   C
ATOM   683 CB  PRO A 88     36.319  59.011  55.857  1.00 19.59      A   C
ATOM   684 CG  PRO A 88     35.648  57.872  56.587  1.00 18.28      A   C
ATOM   685 C   PRO A 88     34.411  60.672  55.577  1.00 19.00      A   C
ATOM   686 O   PRO A 88     33.318  60.125  55.711  1.00 17.80      A   O
ATOM   687 N   ILE A 89     34.622  61.668  54.726  1.00 19.35      A   N
ATOM   688 CA  ILE A 89     33.577  62.163  53.843  1.00 18.35      A   C
ATOM   689 CB  ILE A 89     33.171  63.613  54.196  1.00 18.03      A   C
ATOM   690 CG2 ILE A 89     32.157  64.136  53.185  1.00 16.99      A   C
ATOM   691 CG1 ILE A 89     32.562  63.641  55.598  1.00 18.30      A   C
ATOM   692 CD1 ILE A 89     32.020  64.990  56.011  1.00 26.25      A   C
ATOM   693 C   ILE A 89     34.134  62.108  52.429  1.00 17.01      A   C
ATOM   694 O   ILE A 89     35.206  62.646  52.144  1.00 18.36      A   O
ATOM   695 N   VAL A 90     33.406  61.435  51.551  1.00 15.45      A   N
ATOM   696 CA  VAL A 90     33.829  61.270  50.173  1.00 14.79      A   C
ATOM   697 CB  VAL A 90     33.899  59.779  49.806  1.00 14.33      A   C
ATOM   698 CG1 VAL A 90     34.409  59.605  48.389  1.00 12.10      A   C
ATOM   699 CG2 VAL A 90     34.804  59.055  50.796  1.00 15.51      A   C
ATOM   700 C   VAL A 90     32.858  61.957  49.234  1.00 14.94      A   C
ATOM   701 O   VAL A 90     31.658  61.702  49.283  1.00 15.20      A   O
ATOM   702 N   GLY A 91     33.391  62.830  48.387  1.00 13.93      A   N
ATOM   703 CA  GLY A 91     32.570  63.540  47.427  1.00 14.67      A   C
ATOM   704 C   GLY A 91     32.606  62.829  46.087  1.00 15.17      A   C
ATOM   705 O   GLY A 91     33.262  61.794  45.937  1.00 15.39      A   O
ATOM   706 N   VAL A 92     31.921  63.391  45.101  1.00 13.28      A   N
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Figure 7N

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ATOM   707 CA  VAL A 92     31.871  62.777  43.782  1.00 15.09    A   C
ATOM   708 CB  VAL A 92     30.434  62.762  43.243  1.00 14.78    A   C
ATOM   709 CG1 VAL A 92     29.629  61.703  43.977  1.00 14.03    A   C
ATOM   710 CG2 VAL A 92     29.793  64.135  43.412  1.00 10.70    A   C
ATOM   711 C   VAL A 92     32.770  63.405  42.730  1.00 14.63    A   C
ATOM   712 O   VAL A 92     32.739  63.006  41.567  1.00 17.71    A   O
ATOM   713 N   ILE A 93     33.578  64.378  43.128  1.00 15.55    A   N
ATOM   714 CA  ILE A 93     34.468  65.025  42.176  1.00 16.08    A   C
ATOM   715 CB  ILE A 93     34.684  66.497  42.561  1.00 16.56    A   C
ATOM   716 CG2 ILE A 93     35.653  67.169  41.589  1.00 11.15    A   C
ATOM   717 CG1 ILE A 93     33.329  67.210  42.555  1.00 17.56    A   C
ATOM   718 CD1 ILE A 93     33.385  68.627  43.056  1.00 24.35    A   C
ATOM   719 C   ILE A 93     35.812  64.304  42.032  1.00 15.47    A   C
ATOM   720 O   ILE A 93     36.180  63.904  40.926  1.00 14.93    A   O
ATOM   721 N   GLU A 94     36.536  64.118  43.132  1.00 16.92    A   N
ATOM   722 CA  GLU A 94     37.831  63.446  43.052  1.00 16.92    A   C
ATOM   723 CB  GLU A 94     38.471  63.305  44.434  1.00 20.92    A   C
ATOM   724 CG  GLU A 94     39.894  62.754  44.361  1.00 26.29    A   C
ATOM   725 CD  GLU A 94     40.576  62.678  45.713  1.00 32.62    A   C
ATOM   726 OE1 GLU A 94     40.310  61.723  46.474  1.00 35.02    A   O
ATOM   727 OE2 GLU A 94     41.377  63.588  46.019  1.00 37.91    A   O
ATOM   728 C   GLU A 94     37.745  62.067  42.399  1.00 16.23    A   C
ATOM   729 O   GLU A 94     38.594  61.710  41.578  1.00 12.72    A   O
ATOM   730 N   PRO A 95     36.728  61.263  42.765  1.00 14.67    A   N
ATOM   731 CD  PRO A 95     35.728  61.426  43.835  1.00 11.50    A   C
ATOM   732 CA  PRO A 95     36.612  59.933  42.154  1.00 13.49    A   C
ATOM   733 CB  PRO A 95     35.324  59.385  42.766  1.00 10.50    A   C
ATOM   734 CG  PRO A 95     35.340  59.990  44.132  1.00 13.67    A   C
ATOM   735 C   PRO A 95     36.552  59.995  40.628  1.00 13.36    A   C
ATOM   736 O   PRO A 95     37.111  59.144  39.942  1.00 13.11    A   O
ATOM   737 N   SER A 96     35.868  61.001  40.097  1.00 13.15    A   N
ATOM   738 CA  SER A 96     35.769  61.145  38.652  1.00 13.88    A   C
ATOM   739 CB  SER A 96     34.712  62.190  38.287  1.00 13.27    A   C
ATOM   740 OG  SER A 96     33.415  61.695  38.569  1.00 13.98    A   O
ATOM   741 C   SER A 96     37.121  61.532  38.062  1.00 16.13    A   C
ATOM   742 O   SER A 96     37.482  61.069  36.978  1.00 16.25    A   O
ATOM   743 N   ILE A 97     37.862  62.381  38.774  1.00 16.51    A   N
ATOM   744 CA  ILE A 97     39.181  62.807  38.318  1.00 16.84    A   C
ATOM   745 CB  ILE A 97     39.836  63.786  39.325  1.00 20.72    A   C
ATOM   746 CG2 ILE A 97     41.243  64.165  38.860  1.00 19.14    A   C
ATOM   747 CG1 ILE A 97     38.968  65.039  39.477  1.00 21.89    A   C
ATOM   748 CD1 ILE A 97     38.774  65.827  38.192  1.00 22.65    A   C
ATOM   749 C   ILE A 97     40.070  61.572  38.178  1.00 17.43    A   C
ATOM   750 O   ILE A 97     40.762  61.399  37.171  1.00 16.68    A   O
ATOM   751 N   LEU A 98     40.043  60.716  39.193  1.00 15.65    A   N
ATOM   752 CA  LEU A 98     40.840  59.498  39.182  1.00 18.16    A   C
ATOM   753 CB  LEU A 98     40.749  58.809  40.547  1.00 16.07    A   C
ATOM   754 CG  LEU A 98     41.359  59.641  41.682  1.00 15.84    A   C
ATOM   755 CD1 LEU A 98     41.069  58.980  43.020  1.00 13.47    A   C
ATOM   756 CD2 LEU A 98     42.866  59.788  41.466  1.00 19.12    A   C
ATOM   757 C   LEU A 98     40.374  58.563  38.063  1.00 17.77    A   C
ATOM   758 O   LEU A 98     41.199  57.934  37.389  1.00 16.62    A   O
ATOM   759 N   ALA A 99     39.058  58.485  37.859  1.00 16.23    A   N
ATOM   760 CA  ALA A 99     38.490  57.643  36.807  1.00 18.22    A   C
ATOM   761 CB  ALA A 99     36.962  57.767  36.788  1.00 20.22    A   C
ATOM   762 C   ALA A 99     39.065  58.077  35.462  1.00 17.90    A   C
ATOM   763 O   ALA A 99     39.496  57.246  34.658  1.00 17.01    A   O
ATOM   764 N   ILE A 100    39.067  59.386  35.226  1.00 15.73    A   N
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Figure 7O

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ATOM   765  CA  ILE A 100      39.601  59.939  33.987  1.00 17.26      A   C
ATOM   766  CB  ILE A 100      39.378  61.461  33.932  1.00 12.99      A   C
ATOM   767  CG2 ILE A 100      40.158  62.065  32.772  1.00 16.82      A   C
ATOM   768  CG1 ILE A 100      37.880  61.752  33.795  1.00 15.82      A   C
ATOM   769  CD1 ILE A 100      37.516  63.216  33.925  1.00 14.23      A   C
ATOM   770  C   ILE A 100     41.099  59.640  33.878  1.00 19.31      A   C
ATOM   771  O   ILE A 100     41.594  59.260  32.815  1.00 19.06      A   O
ATOM   772  N   LYS A 101     41.812  59.802  34.986  1.00 19.58      A   N
ATOM   773  CA  LYS A 101      43.246  59.543  35.019  1.00 22.07      A   C
ATOM   774  CB  LYS A 101      43.771  59.741  36.440  1.00 23.70      A   C
ATOM   775  CG  LYS A 101      45.273  59.581  36.595  1.00 28.63      A   C
ATOM   776  CD  LYS A 101      45.671  59.665  38.062  1.00 33.56      A   C
ATOM   777  CE  LYS A 101      47.180  59.570  38.245  1.00 36.39      A   C
ATOM   778  NZ  LYS A 101      47.894  60.739  37.649  1.00 38.26      A   N
ATOM   779  C   LYS A 101     43.538  58.117  34.551  1.00 23.93      A   C
ATOM   780  O   LYS A 101     44.472  57.882  33.780  1.00 23.77      A   O
ATOM   781  N   ARG A 102     42.723  57.174  35.010  1.00 23.37      A   N
ATOM   782  CA  ARG A 102      42.899  55.775  34.655  1.00 25.65      A   C
ATOM   783  CB  ARG A 102      42.096  54.870  35.593  1.00 25.41      A   C
ATOM   784  CG  ARG A 102      42.656  54.749  37.000  1.00 28.61      A   C
ATOM   785  CD  ARG A 102      41.926  53.657  37.782  1.00 31.73      A   C
ATOM   786  NE  ARG A 102      40.486  53.903  37.858  1.00 35.18      A   N
ATOM   787  CZ  ARG A 102      39.903  54.713  38.736  1.00 34.42      A   C
ATOM   788  NH1 ARG A 102      38.586  54.876  38.718  1.00 29.69      A   N
ATOM   789  NH2 ARG A 102      40.637  55.344  39.644  1.00 34.01      A   N
ATOM   790  C   ARG A 102     42.522  55.437  33.222  1.00 26.39      A   C
ATOM   791  O   ARG A 102     43.180  54.611  32.594  1.00 26.86      A   O
ATOM   792  N   GLN A 103     41.473  56.061  32.694  1.00 26.77      A   N
ATOM   793  CA  GLN A 103      41.067  55.733  31.331  1.00 27.82      A   C
ATOM   794  CB  GLN A 103      39.585  55.335  31.306  1.00 28.07      A   C
ATOM   795  CG  GLN A 103      38.661  56.210  32.116  1.00 31.66      A   C
ATOM   796  CD  GLN A 103      37.378  55.489  32.504  1.00 32.01      A   C
ATOM   797  OE1 GLN A 103      36.672  54.951  31.651  1.00 32.82      A   O
ATOM   798  NE2 GLN A 103      37.071  55.479  33.797  1.00 31.78      A   N
ATOM   799  C   GLN A 103     41.363  56.739  30.223  1.00 26.37      A   C
ATOM   800  O   GLN A 103     41.024  56.494  29.066  1.00 26.19      A   O
ATOM   801  N   VAL A 104     42.003  57.856  30.559  1.00 25.47      A   N
ATOM   802  CA  VAL A 104      42.342  58.855  29.550  1.00 24.55      A   C
ATOM   803  CB  VAL A 104      41.542  60.154  29.756  1.00 23.42      A   C
ATOM   804  CG1 VAL A 104      41.998  61.208  28.755  1.00 24.85      A   C
ATOM   805  CG2 VAL A 104      40.055  59.876  29.582  1.00 19.58      A   C
ATOM   806  C   VAL A 104     43.838  59.174  29.578  1.00 26.78      A   C
ATOM   807  O   VAL A 104     44.287  60.043  30.324  1.00 25.34      A   O
ATOM   808  N   GLU A 105     44.601  58.460  28.755  1.00 27.15      A   N
ATOM   809  CA  GLU A 105      46.045  58.641  28.679  1.00 28.29      A   C
ATOM   810  CB  GLU A 105      46.680  57.457  27.947  1.00 33.28      A   C
ATOM   811  CG  GLU A 105      46.743  56.183  28.771  1.00 42.55      A   C
ATOM   812  CD  GLU A 105      47.669  56.315  29.969  1.00 46.07      A   C
ATOM   813  OE1 GLU A 105      47.467  57.242  30.784  1.00 48.67      A   O
ATOM   814  OE2 GLU A 105      48.600  55.491  30.095  1.00 49.87      A   O
ATOM   815  C   GLU A 105     46.461  59.930  27.995  1.00 27.62      A   C
ATOM   816  O   GLU A 105     47.395  60.600  28.437  1.00 27.02      A   O
ATOM   817  N   ASP A 106     45.769  60.273  26.914  1.00 26.11      A   N
ATOM   818  CA  ASP A 106      46.079  61.485  26.164  1.00 25.35      A   C
ATOM   819  CB  ASP A 106      45.271  61.526  24.867  1.00 24.40      A   C
ATOM   820  CG  ASP A 106      45.714  62.641  23.932  1.00 25.06      A   C
ATOM   821  OD1 ASP A 106      46.302  63.640  24.404  1.00 25.51      A   O
ATOM   822  OD2 ASP A 106      45.458  62.522  22.718  1.00 25.51      A   O
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Figure 7P

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ATOM   823  C   ASP A 106     45.759  62.722  26.991  1.00 24.65      A   C
ATOM   824  O   ASP A 106     44.593  63.086  27.142  1.00 24.49      A   O
ATOM   825  N   LYS A 107     46.791  63.372  27.519  1.00 25.06      A   N
ATOM   826  CA  LYS A 107     46.593  64.570  28.327  1.00 24.62      A   C
ATOM   827  CB  LYS A 107     47.919  65.024  28.954  1.00 26.00      A   C
ATOM   828  CG  LYS A 107     48.506  64.047  29.972  1.00 28.40      A   C
ATOM   829  CD  LYS A 107     47.527  63.770  31.107  1.00 26.24      A   C
ATOM   830  CE  LYS A 107     48.086  62.757  32.090  1.00 30.72      A   C
ATOM   831  NZ  LYS A 107     47.086  62.398  33.133  1.00 34.82      A   N
ATOM   832  C   LYS A 107     46.000  65.708  27.503  1.00 24.04      A   C
ATOM   833  O   LYS A 107     45.538  66.706  28.054  1.00 25.01      A   O
ATOM   834  N   ASN A 108     46.014  65.555  26.182  1.00 24.07      A   N
ATOM   835  CA  ASN A 108     45.473  66.572  25.286  1.00 23.49      A   C
ATOM   836  CB  ASN A 108     46.390  66.750  24.073  1.00 23.91      A   C
ATOM   837  CG  ASN A 108     47.596  67.601  24.385  1.00 26.66      A   C
ATOM   838  OD1 ASN A 108     47.464  68.780  24.716  1.00 28.22      A   O
ATOM   839  ND2 ASN A 108     48.780  67.011  24.293  1.00 26.45      A   N
ATOM   840  C   ASN A 108     44.059  66.255  24.818  1.00 21.66      A   C
ATOM   841  O   ASN A 108     43.487  66.983  24.009  1.00 22.58      A   O
ATOM   842  N   ALA A 109     43.494  65.164  25.321  1.00 21.45      A   N
ATOM   843  CA  ALA A 109     42.137  64.793  24.946  1.00 20.49      A   C
ATOM   844  CB  ALA A 109     41.755  63.468  25.599  1.00 21.55      A   C
ATOM   845  C   ALA A 109     41.187  65.902  25.402  1.00 18.98      A   C
ATOM   846  O   ALA A 109     41.237  66.346  26.546  1.00 18.14      A   O
ATOM   847  N   PRO A 110     40.315  66.375  24.505  1.00 19.61      A   N
ATOM   848  CD  PRO A 110     40.090  65.997  23.100  1.00 20.78      A   C
ATOM   849  CA  PRO A 110     39.397  67.436  24.919  1.00 18.53      A   C
ATOM   850  CB  PRO A 110     38.762  67.872  23.606  1.00 18.56      A   C
ATOM   851  CG  PRO A 110     38.726  66.596  22.825  1.00 22.18      A   C
ATOM   852  C   PRO A 110     38.380  66.924  25.928  1.00 17.90      A   C
ATOM   853  O   PRO A 110     37.623  65.996  25.650  1.00 18.78      A   O
ATOM   854  N   ILE A 111     38.384  67.526  27.109  1.00 16.88      A   N
ATOM   855  CA  ILE A 111     37.461  67.137  28.165  1.00 16.87      A   C
ATOM   856  CB  ILE A 111     38.197  66.905  29.503  1.00 17.13      A   C
ATOM   857  CG2 ILE A 111     37.195  66.560  30.592  1.00 18.00      A   C
ATOM   858  CG1 ILE A 111     39.225  65.780  29.352  1.00 16.90      A   C
ATOM   859  CD1 ILE A 111     40.127  65.612  30.574  1.00 20.07      A   C
ATOM   860  C   ILE A 111     36.438  68.246  28.360  1.00 14.74      A   C
ATOM   861  O   ILE A 111     36.792  69.422  28.422  1.00 18.10      A   O
ATOM   862  N   LEU A 112     35.170  67.861  28.450  1.00 15.95      A   N
ATOM   863  CA  LEU A 112     34.086  68.814  28.646  1.00 15.98      A   C
ATOM   864  CB  LEU A 112     33.081  68.715  27.498  1.00 13.81      A   C
ATOM   865  CG  LEU A 112     31.755  69.460  27.703  1.00 17.30      A   C
ATOM   866  CD1 LEU A 112     32.000  70.958  27.834  1.00 12.50      A   C
ATOM   867  CD2 LEU A 112     30.832  69.165  26.524  1.00 17.57      A   C
ATOM   868  C   LEU A 112     33.379  68.527  29.966  1.00 15.50      A   C
ATOM   869  O   LEU A 112     32.823  67.445  30.158  1.00 14.25      A   O
ATOM   870  N   VAL A 113     33.394  69.507  30.864  1.00 15.54      A   N
ATOM   871  CA  VAL A 113     32.767  69.361  32.173  1.00 15.01      A   C
ATOM   872  CB  VAL A 113     33.614  70.035  33.278  1.00 16.33      A   C
ATOM   873  CG1 VAL A 113     33.011  69.752  34.653  1.00 12.34      A   C
ATOM   874  CG2 VAL A 113     35.053  69.538  33.208  1.00 15.51      A   C
ATOM   875  C   VAL A 113     31.390  70.006  32.178  1.00 15.47      A   C
ATOM   876  O   VAL A 113     31.257  71.197  31.901  1.00 15.67      A   O
ATOM   877  N   LEU A 114     30.370  69.215  32.494  1.00 14.67      A   N
ATOM   878  CA  LEU A 114     29.000  69.717  32.554  1.00 13.42      A   C
ATOM   879  CB  LEU A 114     28.074  68.836  31.716  1.00 13.87      A   C
ATOM   880  CG  LEU A 114     28.440  68.622  30.247  1.00 15.67      A   C
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Figure 7Q

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ATOM   881 CD1 LEU A 114     27.349  67.775  29.595  1.00 14.66    A   C
ATOM   882 CD2 LEU A 114     28.583  69.965  29.528  1.00 16.47    A   C
ATOM   883 C   LEU A 114     28.536  69.684  34.006  1.00 12.89    A   C
ATOM   884 O   LEU A 114     28.772  68.706  34.718  1.00 12.06    A   O
ATOM   885 N   GLY A 115     27.873  70.745  34.451  1.00 13.97    A   N
ATOM   886 CA  GLY A 115     27.403  70.763  35.822  1.00 12.19    A   C
ATOM   887 C   GLY A 115     26.528  71.961  36.088  1.00 13.28    A   C
ATOM   888 O   GLY A 115     26.171  72.696  35.160  1.00 14.73    A   O
ATOM   889 N   THR A 116     26.167  72.153  37.351  1.00 11.11    A   N
ATOM   890 CA  THR A 116     25.348  73.297  37.725  1.00 13.32    A   C
ATOM   891 CB  THR A 116     24.866  73.197  39.170  1.00 11.37    A   C
ATOM   892 OG1 THR A 116     26.000  73.180  40.041  1.00 10.70    A   O
ATOM   893 CG2 THR A 116     24.036  71.939  39.367  1.00 10.35    A   C
ATOM   894 C   THR A 116     26.195  74.554  37.614  1.00 14.14    A   C
ATOM   895 O   THR A 116     27.416  74.482  37.431  1.00 14.71    A   O
ATOM   896 N   LYS A 117     25.535  75.701  37.716  1.00 13.99    A   N
ATOM   897 CA  LYS A 117     26.204  76.993  37.657  1.00 14.71    A   C
ATOM   898 CB  LYS A 117     25.147  78.105  37.777  1.00 15.38    A   C
ATOM   899 CG  LYS A 117     25.652  79.472  38.236  1.00 25.83    A   C
ATOM   900 CD  LYS A 117     26.685  80.064  37.296  1.00 33.76    A   C
ATOM   901 CE  LYS A 117     26.103  80.361  35.920  1.00 38.20    A   C
ATOM   902 NZ  LYS A 117     27.105  81.002  35.015  1.00 42.09    A   N
ATOM   903 C   LYS A 117     27.233  77.085  38.787  1.00 12.72    A   C
ATOM   904 O   LYS A 117     28.356  77.549  38.588  1.00 11.82    A   O
ATOM   905 N   ALA A 118     26.854  76.621  39.972  1.00 11.59    A   N
ATOM   906 CA  ALA A 118     27.750  76.671  41.120  1.00 11.90    A   C
ATOM   907 CB  ALA A 118     26.990  76.297  42.382  1.00  8.77    A   C
ATOM   908 C   ALA A 118     28.965  75.758  40.955  1.00 13.39    A   C
ATOM   909 O   ALA A 118     30.099  76.161  41.223  1.00 14.34    A   O
ATOM   910 N   THR A 119     28.721  74.530  40.508  1.00 13.12    A   N
ATOM   911 CA  THR A 119     29.789  73.561  40.316  1.00 12.85    A   C
ATOM   912 CB  THR A 119     29.224  72.205  39.840  1.00 13.42    A   C
ATOM   913 OG1 THR A 119     28.398  71.647  40.869  1.00 11.57    A   O
ATOM   914 CG2 THR A 119     30.353  71.235  39.509  1.00 13.13    A   C
ATOM   915 C   THR A 119     30.808  74.050  39.298  1.00 12.99    A   C
ATOM   916 O   THR A 119     32.016  74.004  39.547  1.00 13.76    A   O
ATOM   917 N   ILE A 120     30.323  74.520  38.154  1.00 11.88    A   N
ATOM   918 CA  ILE A 120     31.213  75.003  37.103  1.00 13.74    A   C
ATOM   919 CB  ILE A 120     30.419  75.310  35.807  1.00 13.41    A   C
ATOM   920 CG2 ILE A 120     31.321  75.980  34.769  1.00 14.31    A   C
ATOM   921 CG1 ILE A 120     29.799  74.012  35.266  1.00 14.49    A   C
ATOM   922 CD1 ILE A 120     30.786  72.862  35.086  1.00 12.48    A   C
ATOM   923 C   ILE A 120     31.977  76.246  37.547  1.00 16.55    A   C
ATOM   924 O   ILE A 120     33.192  76.337  37.372  1.00 18.38    A   O
ATOM   925 N   GLN A 121     31.257  77.200  38.126  1.00 19.17    A   N
ATOM   926 CA  GLN A 121     31.861  78.437  38.601  1.00 20.47    A   C
ATOM   927 CB  GLN A 121     30.790  79.302  39.275  1.00 22.58    A   C
ATOM   928 CG  GLN A 121     31.332  80.406  40.175  1.00 27.23    A   C
ATOM   929 CD  GLN A 121     30.251  81.377  40.627  1.00 30.53    A   C
ATOM   930 OE1 GLN A 121     30.383  82.030  41.664  1.00 32.67    A   O
ATOM   931 NE2 GLN A 121     29.185  81.486  39.842  1.00 28.50    A   N
ATOM   932 C   GLN A 121     33.012  78.170  39.570  1.00 20.02    A   C
ATOM   933 O   GLN A 121     33.979  78.931  39.622  1.00 20.38    A   O
ATOM   934 N   SER A 122     32.905  77.082  40.326  1.00 20.65    A   N
ATOM   935 CA  SER A 122     33.919  76.709  41.311  1.00 19.01    A   C
ATOM   936 CB  SER A 122     33.377  75.609  42.222  1.00 17.57    A   C
ATOM   937 OG  SER A 122     33.446  74.356  41.556  1.00 13.49    A   O
ATOM   938 C   SER A 122     35.220  76.201  40.686  1.00 18.75    A   C
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Figure 7R

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ATOM   939 O   SER A 122    36.270  76.232  41.325  1.00 17.22    A   O
ATOM   940 N   ASN A 123    35.136  75.709  39.454  1.00 18.64    A   N
ATOM   941 CA  ASN A 123    36.292  75.159  38.752  1.00 19.81    A   C
ATOM   942 CB  ASN A 123    37.355  76.237  38.538  1.00 23.62    A   C
ATOM   943 CG  ASN A 123    36.915  77.277  37.537  1.00 27.79    A   C
ATOM   944 OD1 ASN A 123    36.375  76.939  36.483  1.00 25.00    A   O
ATOM   945 ND2 ASN A 123    37.141  78.549  37.855  1.00 30.06    A   N
ATOM   946 C   ASN A 123    36.898  73.967  39.487  1.00 18.35    A   C
ATOM   947 O   ASN A 123    38.057  73.606  39.272  1.00 15.93    A   O
ATOM   948 N   ALA A 124    36.101  73.356  40.356  1.00 16.83    A   N
ATOM   949 CA  ALA A 124    36.550  72.197  41.113  1.00 18.02    A   C
ATOM   950 CB  ALA A 124    35.392  71.613  41.914  1.00 17.02    A   C
ATOM   951 C   ALA A 124    37.109  71.148  40.157  1.00 16.55    A   C
ATOM   952 O   ALA A 124    38.195  70.614  40.376  1.00 17.86    A   O
ATOM   953 N   TYR A 125    36.370  70.858  39.091  1.00 15.55    A   N
ATOM   954 CA  TYR A 125    36.817  69.870  38.121  1.00 15.38    A   C
ATOM   955 CB  TYR A 125    35.699  69.549  37.125  1.00 14.36    A   C
ATOM   956 CG  TYR A 125    34.638  68.609  37.662  1.00 15.54    A   C
ATOM   957 CD1 TYR A 125    33.460  69.096  38.226  1.00 13.69    A   C
ATOM   958 CE1 TYR A 125    32.478  68.230  38.701  1.00 16.51    A   C
ATOM   959 CD2 TYR A 125    34.813  67.224  37.591  1.00 15.03    A   C
ATOM   960 CE2 TYR A 125    33.839  66.349  38.064  1.00 16.83    A   C
ATOM   961 CZ  TYR A 125    32.677  66.857  38.614  1.00 15.95    A   C
ATOM   962 OH  TYR A 125    31.718  65.993  39.065  1.00 16.50    A   O
ATOM   963 C   TYR A 125    38.060  70.323  37.361  1.00 15.65    A   C
ATOM   964 O   TYR A 125    39.050  69.596  37.289  1.00 12.18    A   O
ATOM   965 N   ASP A 126    37.998  71.523  36.796  1.00 15.04    A   N
ATOM   966 CA  ASP A 126    39.110  72.080  36.032  1.00 19.15    A   C
ATOM   967 CB  ASP A 126    38.805  73.530  35.642  1.00 18.87    A   C
ATOM   968 CG  ASP A 126    37.532  73.659  34.831  1.00 21.01    A   C
ATOM   969 OD1 ASP A 126    36.489  73.129  35.271  1.00 22.54    A   O
ATOM   970 OD2 ASP A 126    37.570  74.295  33.756  1.00 22.03    A   O
ATOM   971 C   ASP A 126    40.423  72.028  36.814  1.00 19.26    A   C
ATOM   972 O   ASP A 126    41.432  71.519  36.316  1.00 19.31    A   O
ATOM   973 N   ASN A 127    40.406  72.542  38.040  1.00 18.32    A   N
ATOM   974 CA  ASN A 127    41.613  72.549  38.860  1.00 20.39    A   C
ATOM   975 CB  ASN A 127    41.349  73.226  40.206  1.00 19.27    A   C
ATOM   976 CG  ASN A 127    41.031  74.703  40.067  1.00 23.43    A   C
ATOM   977 OD1 ASN A 127    41.553  75.382  39.185  1.00 25.20    A   O
ATOM   978 ND2 ASN A 127    40.185  75.213  40.955  1.00 22.93    A   N
ATOM   979 C   ASN A 127    42.183  71.155  39.096  1.00 19.69    A   C
ATOM   980 O   ASN A 127    43.381  70.926  38.926  1.00 19.93    A   O
ATOM   981 N   ALA A 128    41.325  70.222  39.488  1.00 17.80    A   N
ATOM   982 CA  ALA A 128    41.767  68.862  39.742  1.00 19.25    A   C
ATOM   983 CB  ALA A 128    40.596  68.016  40.218  1.00 17.14    A   C
ATOM   984 C   ALA A 128    42.383  68.253  38.489  1.00 18.99    A   C
ATOM   985 O   ALA A 128    43.434  67.614  38.553  1.00 21.03    A   O
ATOM   986 N   LEU A 129    41.734  68.456  37.347  1.00 18.35    A   N
ATOM   987 CA  LEU A 129    42.237  67.911  36.088  1.00 18.37    A   C
ATOM   988 CB  LEU A 129    41.229  68.157  34.966  1.00 16.99    A   C
ATOM   989 CG  LEU A 129    39.944  67.331  35.044  1.00 17.37    A   C
ATOM   990 CD1 LEU A 129    38.906  67.908  34.101  1.00 18.55    A   C
ATOM   991 CD2 LEU A 129    40.247  65.878  34.690  1.00 19.31    A   C
ATOM   992 C   LEU A 129    43.586  68.512  35.709  1.00 18.69    A   C
ATOM   993 O   LEU A 129    44.486  67.799  35.264  1.00 16.61    A   O
ATOM   994 N   LYS A 130    43.722  69.823  35.881  1.00 20.51    A   N
ATOM   995 CA  LYS A 130    44.974  70.492  35.559  1.00 25.95    A   C
ATOM   996 CB  LYS A 130    44.869  72.002  35.815  1.00 29.56    A   C
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Figure 7S

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ATOM   997 CG  LYS A 130    44.065  72.756  34.766  1.00 35.38    A   C
ATOM   998 CD  LYS A 130    44.211  74.273  34.910  1.00 40.67    A   C
ATOM   999 CE  LYS A 130    43.491  74.796  36.138  1.00 44.58    A   C
ATOM  1000 NZ  LYS A 130    42.021  74.573  36.036  1.00 48.51    A   N
ATOM  1001 C   LYS A 130    46.084  69.899  36.413  1.00 27.20    A   C
ATOM  1002 O   LYS A 130    47.173  69.607  35.921  1.00 26.83    A   O
ATOM  1003 N   GLN A 131    45.793  69.711  37.695  1.00 27.73    A   N
ATOM  1004 CA  GLN A 131    46.768  69.152  38.615  1.00 30.51    A   C
ATOM  1005 CB  GLN A 131    46.168  69.058  40.017  1.00 34.61    A   C
ATOM  1006 CG  GLN A 131    47.164  68.658  41.086  1.00 44.44    A   C
ATOM  1007 CD  GLN A 131    46.499  68.364  42.414  1.00 49.85    A   C
ATOM  1008 OE1 GLN A 131    45.721  67.415  42.532  1.00 53.57    A   O
ATOM  1009 NE2 GLN A 131    46.797  69.181  43.423  1.00 52.59    A   N
ATOM  1010 C   GLN A 131    47.205  67.769  38.139  1.00 29.59    A   C
ATOM  1011 O   GLN A 131    48.333  67.347  38.389  1.00 27.34    A   O
ATOM  1012 N   GLN A 132    46.311  67.066  37.452  1.00 27.34    A   N
ATOM  1013 CA  GLN A 132    46.634  65.738  36.950  1.00 28.50    A   C
ATOM  1014 CB  GLN A 132    45.382  64.865  36.894  1.00 30.13    A   C
ATOM  1015 CG  GLN A 132    44.863  64.445  38.253  1.00 32.88    A   C
ATOM  1016 CD  GLN A 132    45.924  63.758  39.093  1.00 36.97    A   C
ATOM  1017 OE1 GLN A 132    46.545  62.787  38.659  1.00 36.12    A   O
ATOM  1018 NE2 GLN A 132    46.136  64.262  40.308  1.00 36.40    A   N
ATOM  1019 C   GLN A 132    47.297  65.764  35.579  1.00 26.54    A   C
ATOM  1020 O   GLN A 132    47.465  64.721  34.948  1.00 25.99    A   O
ATOM  1021 N   GLY A 133    47.653  66.958  35.113  1.00 25.65    A   N
ATOM  1022 CA  GLY A 133    48.326  67.079  33.833  1.00 25.61    A   C
ATOM  1023 C   GLY A 133    47.496  67.252  32.575  1.00 26.98    A   C
ATOM  1024 O   GLY A 133    48.061  67.293  31.479  1.00 25.64    A   O
ATOM  1025 N   TYR A 134    46.174  67.353  32.696  1.00 25.10    A   N
ATOM  1026 CA  TYR A 134    45.357  67.526  31.495  1.00 24.59    A   C
ATOM  1027 CB  TYR A 134    43.902  67.120  31.762  1.00 20.44    A   C
ATOM  1028 CG  TYR A 134    43.781  65.626  31.951  1.00 19.78    A   C
ATOM  1029 CD1 TYR A 134    43.870  65.050  33.219  1.00 21.76    A   C
ATOM  1030 CE1 TYR A 134    43.868  63.664  33.380  1.00 19.57    A   C
ATOM  1031 CD2 TYR A 134    43.681  64.774  30.850  1.00 19.08    A   C
ATOM  1032 CE2 TYR A 134    43.682  63.389  31.002  1.00 17.24    A   C
ATOM  1033 CZ  TYR A 134    43.777  62.842  32.265  1.00 18.47    A   C
ATOM  1034 OH  TYR A 134    43.792  61.473  32.413  1.00 19.23    A   O
ATOM  1035 C   TYR A 134    45.461  68.951  30.972  1.00 22.87    A   C
ATOM  1036 O   TYR A 134    45.446  69.908  31.746  1.00 22.48    A   O
ATOM  1037 N   LEU A 135    45.571  69.078  29.650  1.00 22.86    A   N
ATOM  1038 CA  LEU A 135    45.750  70.377  29.008  1.00 24.08    A   C
ATOM  1039 CB  LEU A 135    47.048  70.359  28.192  1.00 24.76    A   C
ATOM  1040 CG  LEU A 135    48.311  69.857  28.906  1.00 25.95    A   C
ATOM  1041 CD1 LEU A 135    49.461  69.790  27.913  1.00 27.98    A   C
ATOM  1042 CD2 LEU A 135    48.658  70.779  30.068  1.00 26.13    A   C
ATOM  1043 C   LEU A 135    44.628  70.873  28.107  1.00 23.53    A   C
ATOM  1044 O   LEU A 135    44.736  71.957  27.539  1.00 24.90    A   O
ATOM  1045 N   ASN A 136    43.556  70.100  27.970  1.00 22.37    A   N
ATOM  1046 CA  ASN A 136    42.450  70.499  27.102  1.00 20.74    A   C
ATOM  1047 CB  ASN A 136    42.411  69.585  25.876  1.00 21.50    A   C
ATOM  1048 CG  ASN A 136    41.613  70.170  24.735  1.00 23.18    A   C
ATOM  1049 OD1 ASN A 136    40.590  70.822  24.945  1.00 25.29    A   O
ATOM  1050 ND2 ASN A 136    42.068  69.923  23.511  1.00 23.17    A   N
ATOM  1051 C   ASN A 136    41.146  70.370  27.887  1.00 20.55    A   C
ATOM  1052 O   ASN A 136    40.430  69.386  27.744  1.00 20.93    A   O
ATOM  1053 N   ILE A 137    40.847  71.371  28.709  1.00 19.65    A   N
ATOM  1054 CA  ILE A 137    39.649  71.347  29.545  1.00 19.51    A   C
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Figure 7T

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ATOM  1055  CB  ILE A 137     40.021  71.504  31.032  1.00 19.77      A   C
ATOM  1056  CG2 ILE A 137     38.792  71.235  31.905  1.00 18.91      A   C
ATOM  1057  CG1 ILE A 137     41.165  70.548  31.388  1.00 17.50      A   C
ATOM  1058  CD1 ILE A 137     41.841  70.877  32.705  1.00 17.99      A   C
ATOM  1059  C   ILE A 137     38.650  72.445  29.214  1.00 18.94      A   C
ATOM  1060  O   ILE A 137     39.008  73.618  29.141  1.00 18.47      A   O
ATOM  1061  N   SER A 138     37.394  72.054  29.019  1.00 18.59      A   N
ATOM  1062  CA  SER A 138     36.319  73.000  28.729  1.00 19.77      A   C
ATOM  1063  CB  SER A 138     35.810  72.829  27.294  1.00 21.73      A   C
ATOM  1064  OG  SER A 138     36.823  73.104  26.345  1.00 24.47      A   O
ATOM  1065  C   SER A 138     35.177  72.716  29.698  1.00 19.64      A   C
ATOM  1066  O   SER A 138     34.971  71.569  30.102  1.00 20.10      A   O
ATOM  1067  N   HIS A 139     34.443  73.753  30.083  1.00 18.51      A   N
ATOM  1068  CA  HIS A 139     33.319  73.565  30.993  1.00 18.98      A   C
ATOM  1069  CB  HIS A 139     33.697  73.982  32.418  1.00 18.17      A   C
ATOM  1070  CG  HIS A 139     34.220  75.380  32.522  1.00 19.94      A   C
ATOM  1071  CD2 HIS A 139     33.634  76.575  32.268  1.00 20.85      A   C
ATOM  1072  ND1 HIS A 139     35.506  75.661  32.926  1.00 20.98      A   N
ATOM  1073  CE1 HIS A 139     35.692  76.970  32.916  1.00 24.03      A   C
ATOM  1074  NE2 HIS A 139     34.572  77.547  32.520  1.00 22.03      A   N
ATOM  1075  C   HIS A 139     32.082  74.329  30.552  1.00 18.46      A   C
ATOM  1076  O   HIS A 139     32.181  75.372  29.909  1.00 19.58      A   O
ATOM  1077  N   LEU A 140     30.918  73.791  30.902  1.00 18.71      A   N
ATOM  1078  CA  LEU A 140     29.634  74.403  30.573  1.00 19.01      A   C
ATOM  1079  CB  LEU A 140     29.028  73.775  29.316  1.00 20.85      A   C
ATOM  1080  CG  LEU A 140     29.476  74.190  27.918  1.00 22.92      A   C
ATOM  1081  CD1 LEU A 140     28.667  73.394  26.904  1.00 21.79      A   C
ATOM  1082  CD2 LEU A 140     29.255  75.688  27.709  1.00 25.42      A   C
ATOM  1083  C   LEU A 140     28.632  74.227  31.702  1.00 17.69      A   C
ATOM  1084  O   LEU A 140     28.422  73.118  32.194  1.00 17.06      A   O
ATOM  1085  N   ALA A 141     28.008  75.322  32.112  1.00 18.99      A   N
ATOM  1086  CA  ALA A 141     26.995  75.256  33.153  1.00 18.92      A   C
ATOM  1087  CB  ALA A 141     26.976  76.553  33.955  1.00 19.92      A   C
ATOM  1088  C   ALA A 141     25.653  75.046  32.456  1.00 20.05      A   C
ATOM  1089  O   ALA A 141     25.002  76.007  32.053  1.00 22.92      A   O
ATOM  1090  N   THR A 142     25.250  73.790  32.299  1.00 17.67      A   N
ATOM  1091  CA  THR A 142     23.983  73.456  31.650  1.00 15.92      A   C
ATOM  1092  CB  THR A 142     24.069  72.061  30.991  1.00 15.55      A   C
ATOM  1093  OG1 THR A 142     24.474  71.094  31.969  1.00 15.28      A   O
ATOM  1094  CG2 THR A 142     25.091  72.069  29.862  1.00 16.16      A   C
ATOM  1095  C   THR A 142     22.890  73.462  32.725  1.00 16.51      A   C
ATOM  1096  O   THR A 142     22.195  72.469  32.942  1.00 15.07      A   O
ATOM  1097  N   SER A 143     22.746  74.608  33.382  1.00 15.40      A   N
ATOM  1098  CA  SER A 143     21.797  74.779  34.479  1.00 16.69      A   C
ATOM  1099  CB  SER A 143     21.745  76.254  34.886  1.00 18.40      A   C
ATOM  1100  OG  SER A 143     20.979  76.419  36.068  1.00 19.14      A   O
ATOM  1101  C   SER A 143     20.374  74.259  34.266  1.00 16.28      A   C
ATOM  1102  O   SER A 143     19.838  73.555  35.119  1.00 17.50      A   O
ATOM  1103  N   LEU A 144     19.766  74.597  33.133  1.00 15.61      A   N
ATOM  1104  CA  LEU A 144     18.397  74.174  32.850  1.00 16.29      A   C
ATOM  1105  CB  LEU A 144     17.920  74.855  31.567  1.00 18.23      A   C
ATOM  1106  CG  LEU A 144     17.915  76.379  31.743  1.00 21.65      A   C
ATOM  1107  CD1 LEU A 144     17.543  77.079  30.440  1.00 21.02      A   C
ATOM  1108  CD2 LEU A 144     16.931  76.741  32.854  1.00 19.77      A   C
ATOM  1109  C   LEU A 144     18.171  72.657  32.772  1.00 15.16      A   C
ATOM  1110  O   LEU A 144     17.036  72.184  32.874  1.00 13.64      A   O
ATOM  1111  N   PHE A 145     19.238  71.888  32.600  1.00 13.93      A   N
ATOM  1112  CA  PHE A 145     19.080  70.437  32.545  1.00 11.95      A   C
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Figure 7U

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ATOM  1113  CB  PHE A 145      20.436  69.742  32.374  1.00 13.43      A   C
ATOM  1114  CG  PHE A 145      21.000  69.808  30.976  1.00 17.43      A   C
ATOM  1115  CD1 PHE A 145      22.248  69.260  30.703  1.00 15.45      A   C
ATOM  1116  CD2 PHE A 145      20.287  70.399  29.933  1.00 17.04      A   C
ATOM  1117  CE1 PHE A 145      22.783  69.295  29.420  1.00 18.35      A   C
ATOM  1118  CE2 PHE A 145      20.815  70.440  28.642  1.00 15.38      A   C
ATOM  1119  CZ  PHE A 145      22.064  69.889  28.385  1.00 16.89      A   C
ATOM  1120  C   PHE A 145      18.436  69.956  33.846  1.00 12.03      A   C
ATOM  1121  O   PHE A 145      17.600  69.064  33.839  1.00 11.95      A   O
ATOM  1122  N   VAL A 146      18.813  70.564  34.965  1.00 12.43      A   N
ATOM  1123  CA  VAL A 146      18.269  70.150  36.255  1.00 11.55      A   C
ATOM  1124  CB  VAL A 146      18.931  70.941  37.420  1.00 11.44      A   C
ATOM  1125  CG1 VAL A 146      18.203  70.669  38.739  1.00 12.27      A   C
ATOM  1126  CG2 VAL A 146      20.389  70.523  37.541  1.00 12.17      A   C
ATOM  1127  C   VAL A 146      16.741  70.243  36.344  1.00 13.17      A   C
ATOM  1128  O   VAL A 146      16.081  69.236  36.566  1.00 13.35      A   O
ATOM  1129  N   PRO A 147      16.157  71.442  36.168  1.00 14.55      A   N
ATOM  1130  CD  PRO A 147      16.725  72.794  36.014  1.00 12.51      A   C
ATOM  1131  CA  PRO A 147      14.693  71.491  36.260  1.00 15.45      A   C
ATOM  1132  CB  PRO A 147      14.386  72.995  36.197  1.00 16.91      A   C
ATOM  1133  CG  PRO A 147      15.556  73.569  35.463  1.00 13.21      A   C
ATOM  1134  C   PRO A 147      13.972  70.682  35.178  1.00 13.90      A   C
ATOM  1135  O   PRO A 147      12.910  70.111  35.433  1.00 15.62      A   O
ATOM  1136  N   LEU A 148      14.549  70.614  33.982  1.00 11.79      A   N
ATOM  1137  CA  LEU A 148      13.929  69.844  32.911  1.00 13.83      A   C
ATOM  1138  CB  LEU A 148      14.748  69.947  31.620  1.00 15.89      A   C
ATOM  1139  CG  LEU A 148      14.193  70.877  30.540  1.00 14.82      A   C
ATOM  1140  CD1 LEU A 148      14.146  72.296  31.057  1.00 18.80      A   C
ATOM  1141  CD2 LEU A 148      15.070  70.792  29.300  1.00 16.16      A   C
ATOM  1142  C   LEU A 148      13.833  68.389  33.336  1.00 13.84      A   C
ATOM  1143  O   LEU A 148      12.786  67.755  33.204  1.00 15.22      A   O
ATOM  1144  N   ILE A 149      14.935  67.872  33.861  1.00 12.81      A   N
ATOM  1145  CA  ILE A 149      14.985  66.493  34.312  1.00 13.21      A   C
ATOM  1146  CB  ILE A 149      16.425  66.111  34.703  1.00 14.51      A   C
ATOM  1147  CG2 ILE A 149      16.444  64.756  35.402  1.00 12.63      A   C
ATOM  1148  CG1 ILE A 149      17.291  66.093  33.434  1.00 15.10      A   C
ATOM  1149  CD1 ILE A 149      18.777  65.893  33.673  1.00 10.57      A   C
ATOM  1150  C   ILE A 149      14.026  66.258  35.470  1.00 14.45      A   C
ATOM  1151  O   ILE A 149      13.425  65.195  35.571  1.00 15.79      A   O
ATOM  1152  N   GLU A 150      13.859  67.256  36.328  1.00 14.06      A   N
ATOM  1153  CA  GLU A 150      12.943  67.121  37.449  1.00 15.01      A   C
ATOM  1154  CB  GLU A 150      13.206  68.228  38.466  1.00 18.77      A   C
ATOM  1155  CG  GLU A 150      14.447  67.930  39.291  1.00 26.06      A   C
ATOM  1156  CD  GLU A 150      14.824  69.044  40.227  1.00 28.16      A   C
ATOM  1157  OE1 GLU A 150      15.731  68.821  41.056  1.00 26.46      A   O
ATOM  1158  OE2 GLU A 150      14.222  70.138  40.128  1.00 31.52      A   O
ATOM  1159  C   GLU A 150      11.481  67.116  37.000  1.00 15.40      A   C
ATOM  1160  O   GLU A 150      10.615  66.617  37.719  1.00 14.17      A   O
ATOM  1161  N   GLU A 151      11.212  67.680  35.822  1.00 13.23      A   N
ATOM  1162  CA  GLU A 151       9.860  67.703  35.265  1.00 15.55      A   C
ATOM  1163  CB  GLU A 151       9.619  68.971  34.442  1.00 16.54      A   C
ATOM  1164  CG  GLU A 151       9.533  70.248  35.267  1.00 20.37      A   C
ATOM  1165  CD  GLU A 151       8.528  70.151  36.401  1.00 23.39      A   C
ATOM  1166  OE1 GLU A 151       7.332  69.901  36.134  1.00 24.54      A   O
ATOM  1167  OE2 GLU A 151       8.937  70.326  37.566  1.00 27.18      A   O
ATOM  1168  C   GLU A 151       9.687  66.487  34.368  1.00 17.22      A   C
ATOM  1169  O   GLU A 151       8.668  66.331  33.687  1.00 16.37      A   O
ATOM  1170  N   SER A 152      10.702  65.632  34.376  1.00 18.04      A   N
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Figure 7V

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ATOM  1171  CA  SER A 152     10.722  64.413  33.578  1.00 18.02      A   C
ATOM  1172  CB  SER A 152      9.559  63.493  33.949  1.00 19.94      A   C
ATOM  1173  OG  SER A 152      9.768  62.207  33.390  1.00 18.81      A   O
ATOM  1174  C   SER A 152     10.699  64.673  32.081  1.00 20.44      A   C
ATOM  1175  O   SER A 152     10.013  63.980  31.323  1.00 22.59      A   O
ATOM  1176  N   ILE A 153     11.443  65.682  31.653  1.00 19.73      A   N
ATOM  1177  CA  ILE A 153     11.541  65.998  30.239  1.00 21.13      A   C
ATOM  1178  CB  ILE A 153     11.541  67.521  30.016  1.00 23.26      A   C
ATOM  1179  CG2 ILE A 153     11.800  67.846  28.546  1.00 22.78      A   C
ATOM  1180  CG1 ILE A 153     10.190  68.086  30.474  1.00 25.17      A   C
ATOM  1181  CD1 ILE A 153     10.005  69.547  30.207  1.00 30.23      A   C
ATOM  1182  C   ILE A 153     12.865  65.372  29.832  1.00 21.67      A   C
ATOM  1183  O   ILE A 153     13.900  66.037  29.784  1.00 20.32      A   O
ATOM  1184  N   LEU A 154     12.811  64.069  29.565  1.00 18.75      A   N
ATOM  1185  CA  LEU A 154     13.986  63.281  29.218  1.00 20.85      A   C
ATOM  1186  CB  LEU A 154     13.939  61.972  30.003  1.00 21.22      A   C
ATOM  1187  CG  LEU A 154     13.540  62.197  31.467  1.00 22.53      A   C
ATOM  1188  CD1 LEU A 154     13.353  60.868  32.182  1.00 21.31      A   C
ATOM  1189  CD2 LEU A 154     14.604  63.040  32.154  1.00 20.71      A   C
ATOM  1190  C   LEU A 154     14.131  62.994  27.726  1.00 21.27      A   C
ATOM  1191  O   LEU A 154     14.969  62.194  27.313  1.00 20.75      A   O
ATOM  1192  N   GLU A 155     13.302  63.649  26.927  1.00 23.77      A   N
ATOM  1193  CA  GLU A 155     13.333  63.499  25.478  1.00 26.10      A   C
ATOM  1194  CB  GLU A 155     12.948  62.069  25.074  1.00 30.66      A   C
ATOM  1195  CG  GLU A 155     11.661  61.554  25.686  1.00 38.37      A   C
ATOM  1196  CD  GLU A 155     10.445  61.898  24.860  1.00 42.76      A   C
ATOM  1197  OE1 GLU A 155      9.322  61.571  25.299  1.00 48.12      A   O
ATOM  1198  OE2 GLU A 155     10.609  62.488  23.771  1.00 46.52      A   O
ATOM  1199  C   GLU A 155     12.366  64.517  24.893  1.00 24.72      A   C
ATOM  1200  O   GLU A 155     11.759  65.288  25.633  1.00 23.59      A   O
ATOM  1201  N   GLY A 156     12.236  64.538  23.573  1.00 23.02      A   N
ATOM  1202  CA  GLY A 156     11.333  65.492  22.958  1.00 21.08      A   C
ATOM  1203  C   GLY A 156     12.047  66.742  22.485  1.00 22.30      A   C
ATOM  1204  O   GLY A 156     13.243  66.925  22.728  1.00 21.15      A   O
ATOM  1205  N   GLU A 157     11.299  67.612  21.817  1.00 20.99      A   N
ATOM  1206  CA  GLU A 157     11.847  68.844  21.268  1.00 22.12      A   C
ATOM  1207  CB  GLU A 157     10.786  69.539  20.412  1.00 25.41      A   C
ATOM  1208  CG  GLU A 157     11.366  70.505  19.398  1.00 32.26      A   C
ATOM  1209  CD  GLU A 157     10.304  71.341  18.720  1.00 37.00      A   C
ATOM  1210  OE1 GLU A 157      9.332  70.758  18.186  1.00 41.42      A   O
ATOM  1211  OE2 GLU A 157     10.443  72.583  18.719  1.00 39.91      A   O
ATOM  1212  C   GLU A 157     12.386  69.835  22.302  1.00 19.65      A   C
ATOM  1213  O   GLU A 157     13.377  70.518  22.053  1.00 18.65      A   O
ATOM  1214  N   LEU A 158     11.734  69.925  23.453  1.00 18.49      A   N
ATOM  1215  CA  LEU A 158     12.172  70.861  24.485  1.00 20.02      A   C
ATOM  1216  CB  LEU A 158     11.174  70.870  25.653  1.00 19.53      A   C
ATOM  1217  CG  LEU A 158     11.410  71.891  26.773  1.00 21.01      A   C
ATOM  1218  CD1 LEU A 158     11.661  73.280  26.191  1.00 20.32      A   C
ATOM  1219  CD2 LEU A 158     10.197  71.910  27.697  1.00 19.63      A   C
ATOM  1220  C   LEU A 158     13.581  70.529  24.976  1.00 17.50      A   C
ATOM  1221  O   LEU A 158     14.424  71.417  25.101  1.00 17.99      A   O
ATOM  1222  N   LEU A 159     13.846  69.253  25.240  1.00 18.72      A   N
ATOM  1223  CA  LEU A 159     15.180  68.856  25.693  1.00 17.84      A   C
ATOM  1224  CB  LEU A 159     15.202  67.377  26.105  1.00 17.62      A   C
ATOM  1225  CG  LEU A 159     16.585  66.818  26.488  1.00 16.01      A   C
ATOM  1226  CD1 LEU A 159     17.125  67.557  27.713  1.00 16.76      A   C
ATOM  1227  CD2 LEU A 159     16.478  65.324  26.775  1.00 16.92      A   C
ATOM  1228  C   LEU A 159     16.185  69.091  24.571  1.00 18.06      A   C
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Figure 7W

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ATOM  1229  O   LEU A 159     17.274  69.629  24.792  1.00 15.90      A   O
ATOM  1230  N   GLU A 160     15.805  68.686  23.363  1.00 17.23      A   N
ATOM  1231  CA  GLU A 160     16.660  68.846  22.199  1.00 19.74      A   C
ATOM  1232  CB  GLU A 160     15.936  68.322  20.951  1.00 22.63      A   C
ATOM  1233  CG  GLU A 160     16.613  68.624  19.612  1.00 25.09      A   C
ATOM  1234  CD  GLU A 160     18.020  68.058  19.496  1.00 28.46      A   C
ATOM  1235  OE1 GLU A 160     18.320  67.041  20.156  1.00 24.99      A   O
ATOM  1236  OE2 GLU A 160     18.824  68.626  18.725  1.00 29.33      A   O
ATOM  1237  C   GLU A 160     17.025  70.316  22.023  1.00 17.75      A   C
ATOM  1238  O   GLU A 160     18.188  70.655  21.795  1.00 17.75      A   O
ATOM  1239  N   THR A 161     16.031  71.188  22.140  1.00 15.91      A   N
ATOM  1240  CA  THR A 161     16.274  72.615  21.984  1.00 17.08      A   C
ATOM  1241  CB  THR A 161     14.955  73.402  21.946  1.00 19.03      A   C
ATOM  1242  OG1 THR A 161     14.165  72.943  20.841  1.00 18.83      A   O
ATOM  1243  CG2 THR A 161     15.225  74.888  21.770  1.00 18.63      A   C
ATOM  1244  C   THR A 161     17.159  73.154  23.104  1.00 16.80      A   C
ATOM  1245  O   THR A 161     17.998  74.029  22.875  1.00 16.81      A   O
ATOM  1246  N   CYS A 162     16.977  72.623  24.309  1.00 15.47      A   N
ATOM  1247  CA  CYS A 162     17.772  73.054  25.451  1.00 16.48      A   C
ATOM  1248  CB  CYS A 162     17.217  72.456  26.748  1.00 17.44      A   C
ATOM  1249  SG  CYS A 162     17.994  73.125  28.246  1.00 17.16      A   S
ATOM  1250  C   CYS A 162     19.226  72.624  25.264  1.00 16.12      A   C
ATOM  1251  O   CYS A 162     20.148  73.390  25.547  1.00 15.64      A   O
ATOM  1252  N   MET A 163     19.433  71.395  24.797  1.00 16.12      A   N
ATOM  1253  CA  MET A 163     20.792  70.913  24.578  1.00 16.90      A   C
ATOM  1254  CB  MET A 163     20.796  69.446  24.152  1.00 17.54      A   C
ATOM  1255  CG  MET A 163     20.259  68.491  25.198  1.00 18.15      A   C
ATOM  1256  SD  MET A 163     20.679  66.775  24.864  1.00 18.78      A   S
ATOM  1257  CE  MET A 163     19.539  66.408  23.514  1.00 18.51      A   C
ATOM  1258  C   MET A 163     21.427  71.760  23.483  1.00 16.80      A   C
ATOM  1259  O   MET A 163     22.601  72.109  23.554  1.00 17.90      A   O
ATOM  1260  N   HIS A 164     20.637  72.083  22.467  1.00 17.35      A   N
ATOM  1261  CA  HIS A 164     21.119  72.893  21.359  1.00 18.77      A   C
ATOM  1262  CB  HIS A 164     20.009  73.065  20.317  1.00 21.03      A   C
ATOM  1263  CG  HIS A 164     20.451  73.784  19.082  1.00 26.61      A   C
ATOM  1264  CD2 HIS A 164     20.862  73.317  17.879  1.00 27.02      A   C
ATOM  1265  ND1 HIS A 164     20.559  75.156  19.018  1.00 26.82      A   N
ATOM  1266  CE1 HIS A 164     21.020  75.503  17.829  1.00 28.20      A   C
ATOM  1267  NE2 HIS A 164     21.212  74.406  17.119  1.00 26.69      A   N
ATOM  1268  C   HIS A 164     21.573  74.249  21.872  1.00 17.93      A   C
ATOM  1269  O   HIS A 164     22.630  74.758  21.483  1.00 18.32      A   O
ATOM  1270  N   TYR A 165     20.775  74.821  22.765  1.00 16.78      A   N
ATOM  1271  CA  TYR A 165     21.073  76.120  23.352  1.00 17.03      A   C
ATOM  1272  CB  TYR A 165     20.004  76.486  24.383  1.00 16.70      A   C
ATOM  1273  CG  TYR A 165     20.323  77.728  25.186  1.00 14.36      A   C
ATOM  1274  CD1 TYR A 165     20.249  78.998  24.611  1.00 18.03      A   C
ATOM  1275  CE1 TYR A 165     20.567  80.144  25.350  1.00 17.68      A   C
ATOM  1276  CD2 TYR A 165     20.722  77.633  26.518  1.00 15.98      A   C
ATOM  1277  CE2 TYR A 165     21.042  78.767  27.263  1.00 15.67      A   C
ATOM  1278  CZ  TYR A 165     20.964  80.015  26.675  1.00 17.67      A   C
ATOM  1279  OH  TYR A 165     21.296  81.128  27.414  1.00 19.35      A   O
ATOM  1280  C   TYR A 165     22.440  76.144  24.025  1.00 18.18      A   C
ATOM  1281  O   TYR A 165     23.202  77.089  23.848  1.00 18.56      A   O
ATOM  1282  N   TYR A 166     22.745  75.101  24.795  1.00 16.65      A   N
ATOM  1283  CA  TYR A 166     24.016  75.022  25.516  1.00 16.14      A   C
ATOM  1284  CB  TYR A 166     23.879  74.113  26.745  1.00 15.22      A   C
ATOM  1285  CG  TYR A 166     23.063  74.681  27.887  1.00 14.44      A   C
ATOM  1286  CD1 TYR A 166     21.955  73.994  28.380  1.00 13.39      A   C
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Figure 7X

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ATOM  1287 CE1 TYR A 166    21.202  74.506  29.438  1.00 14.31    A   C
ATOM  1288 CD2 TYR A 166    23.403  75.898  28.481  1.00 14.07    A   C
ATOM  1289 CE2 TYR A 166    22.660  76.419  29.537  1.00 13.27    A   C
ATOM  1290 CZ  TYR A 166    21.558  75.717  30.008  1.00 15.59    A   C
ATOM  1291 OH  TYR A 166    20.800  76.228  31.033  1.00 13.70    A   O
ATOM  1292 C   TYR A 166    25.207  74.520  24.710  1.00 16.15    A   C
ATOM  1293 O   TYR A 166    26.320  75.020  24.862  1.00 18.32    A   O
ATOM  1294 N   PHE A 167    24.977  73.532  23.858  1.00 16.40    A   N
ATOM  1295 CA  PHE A 167    26.063  72.926  23.099  1.00 19.32    A   C
ATOM  1296 CB  PHE A 167    25.696  71.466  22.811  1.00 18.55    A   C
ATOM  1297 CG  PHE A 167    25.487  70.633  24.056  1.00 17.57    A   C
ATOM  1298 CD1 PHE A 167    24.611  69.551  24.044  1.00 17.73    A   C
ATOM  1299 CD2 PHE A 167    26.179  70.920  25.232  1.00 17.53    A   C
ATOM  1300 CE1 PHE A 167    24.429  68.766  25.186  1.00 17.59    A   C
ATOM  1301 CE2 PHE A 167    26.005  70.140  26.378  1.00 15.09    A   C
ATOM  1302 CZ  PHE A 167    25.130  69.063  26.354  1.00 15.31    A   C
ATOM  1303 C   PHE A 167    26.517  73.613  21.810  1.00 21.91    A   C
ATOM  1304 O   PHE A 167    27.693  73.529  21.444  1.00 18.63    A   O
ATOM  1305 N   THR A 168    25.600  74.293  21.128  1.00 23.53    A   N
ATOM  1306 CA  THR A 168    25.940  74.958  19.871  1.00 25.11    A   C
ATOM  1307 CB  THR A 168    24.757  75.788  19.346  1.00 24.47    A   C
ATOM  1308 OG1 THR A 168    23.646  74.919  19.099  1.00 28.03    A   O
ATOM  1309 CG2 THR A 168    25.133  76.488  18.048  1.00 28.49    A   C
ATOM  1310 C   THR A 168    27.182  75.849  19.920  1.00 24.43    A   C
ATOM  1311 O   THR A 168    27.989  75.836  18.995  1.00 26.62    A   O
ATOM  1312 N   PRO A 169    27.347  76.640  20.992  1.00 25.87    A   N
ATOM  1313 CD  PRO A 169    26.337  76.983  22.009  1.00 23.89    A   C
ATOM  1314 CA  PRO A 169    28.512  77.523  21.113  1.00 28.42    A   C
ATOM  1315 CB  PRO A 169    28.198  78.329  22.372  1.00 25.95    A   C
ATOM  1316 CG  PRO A 169    26.709  78.406  22.351  1.00 26.22    A   C
ATOM  1317 C   PRO A 169    29.868  76.813  21.210  1.00 30.41    A   C
ATOM  1318 O   PRO A 169    30.914  77.440  21.035  1.00 30.45    A   O
ATOM  1319 N   LEU A 170    29.853  75.512  21.487  1.00 32.27    A   N
ATOM  1320 CA  LEU A 170    31.094  74.755  21.611  1.00 34.59    A   C
ATOM  1321 CB  LEU A 170    30.808  73.338  22.098  1.00 33.83    A   C
ATOM  1322 CG  LEU A 170    30.417  73.202  23.568  1.00 32.01    A   C
ATOM  1323 CD1 LEU A 170    30.035  71.760  23.848  1.00 29.69    A   C
ATOM  1324 CD2 LEU A 170    31.579  73.641  24.458  1.00 29.22    A   C
ATOM  1325 C   LEU A 170    31.897  74.677  20.323  1.00 37.74    A   C
ATOM  1326 O   LEU A 170    31.358  74.386  19.254  1.00 39.31    A   O
ATOM  1327 N   GLU A 171    33.197  74.924  20.434  1.00 40.03    A   N
ATOM  1328 CA  GLU A 171    34.076  74.871  19.276  1.00 43.34    A   C
ATOM  1329 CB  GLU A 171    34.750  76.229  19.067  1.00 48.27    A   C
ATOM  1330 CG  GLU A 171    33.759  77.349  18.782  1.00 54.56    A   C
ATOM  1331 CD  GLU A 171    33.072  77.200  17.431  1.00 59.45    A   C
ATOM  1332 OE1 GLU A 171    32.919  76.051  16.953  1.00 60.27    A   O
ATOM  1333 OE2 GLU A 171    32.672  78.237  16.852  1.00 61.77    A   O
ATOM  1334 C   GLU A 171    35.120  73.777  19.447  1.00 42.59    A   C
ATOM  1335 O   GLU A 171    36.239  73.888  18.951  1.00 43.77    A   O
ATOM  1336 N   ILE A 172    34.741  72.717  20.155  1.00 40.35    A   N
ATOM  1337 CA  ILE A 172    35.636  71.589  20.391  1.00 38.22    A   C
ATOM  1338 CB  ILE A 172    36.155  71.569  21.842  1.00 37.75    A   C
ATOM  1339 CG2 ILE A 172    36.806  72.901  22.184  1.00 34.13    A   C
ATOM  1340 CG1 ILE A 172    34.997  71.276  22.797  1.00 36.28    A   C
ATOM  1341 CD1 ILE A 172    35.430  70.993  24.225  1.00 40.90    A   C
ATOM  1342 C   ILE A 172    34.911  70.272  20.145  1.00 36.42    A   C
ATOM  1343 O   ILE A 172    33.688  70.200  20.222  1.00 39.20    A   O
ATOM  1344 N   LEU A 173    35.674  69.231  19.838  1.00 34.80    A   N
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Figure 7Y

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ATOM  1345  CA  LEU A 173      35.104  67.910  19.612  1.00 32.15      A   C
ATOM  1346  CB  LEU A 173      35.718  67.265  18.363  1.00 33.04      A   C
ATOM  1347  CG  LEU A 173      35.480  67.998  17.037  1.00 34.61      A   C
ATOM  1348  CD1 LEU A 173      36.221  67.290  15.910  1.00 33.74      A   C
ATOM  1349  CD2 LEU A 173      33.979  68.056  16.747  1.00 34.77      A   C
ATOM  1350  C   LEU A 173      35.454  67.102  20.855  1.00 29.45      A   C
ATOM  1351  O   LEU A 173      36.481  66.424  20.896  1.00 27.62      A   O
ATOM  1352  N   PRO A 174      34.598  67.167  21.891  1.00 27.18      A   N
ATOM  1353  CD  PRO A 174      33.272  67.811  21.931  1.00 26.43      A   C
ATOM  1354  CA  PRO A 174      34.858  66.432  23.132  1.00 24.33      A   C
ATOM  1355  CB  PRO A 174      33.646  66.772  24.003  1.00 25.04      A   C
ATOM  1356  CG  PRO A 174      32.560  67.015  22.997  1.00 27.39      A   C
ATOM  1357  C   PRO A 174      35.067  64.934  22.991  1.00 21.39      A   C
ATOM  1358  O   PRO A 174      34.335  64.250  22.277  1.00 22.17      A   O
ATOM  1359  N   GLU A 175      36.088  64.438  23.679  1.00 19.42      A   N
ATOM  1360  CA  GLU A 175      36.405  63.021  23.683  1.00 19.85      A   C
ATOM  1361  CB  GLU A 175      37.905  62.821  23.465  1.00 21.90      A   C
ATOM  1362  CG  GLU A 175      38.320  62.869  21.999  1.00 27.70      A   C
ATOM  1363  CD  GLU A 175      39.823  62.943  21.802  1.00 27.64      A   C
ATOM  1364  OE1 GLU A 175      40.565  62.242  22.523  1.00 28.19      A   O
ATOM  1365  OE2 GLU A 175      40.260  63.701  20.913  1.00 30.42      A   O
ATOM  1366  C   GLU A 175      35.983  62.473  25.044  1.00 19.80      A   C
ATOM  1367  O   GLU A 175      35.855  61.263  25.239  1.00 19.75      A   O
ATOM  1368  N   VAL A 176      35.762  63.383  25.986  1.00 18.80      A   N
ATOM  1369  CA  VAL A 176      35.349  63.006  27.330  1.00 17.58      A   C
ATOM  1370  CB  VAL A 176      36.550  62.981  28.313  1.00 16.92      A   C
ATOM  1371  CG1 VAL A 176      36.091  62.488  29.676  1.00 15.99      A   C
ATOM  1372  CG2 VAL A 176      37.661  62.087  27.772  1.00 16.67      A   C
ATOM  1373  C   VAL A 176      34.330  64.014  27.840  1.00 16.96      A   C
ATOM  1374  O   VAL A 176      34.533  65.224  27.746  1.00 17.95      A   O
ATOM  1375  N   ILE A 177      33.222  63.509  28.362  1.00 17.35      A   N
ATOM  1376  CA  ILE A 177      32.184  64.373  28.902  1.00 15.36      A   C
ATOM  1377  CB  ILE A 177      30.873  64.272  28.100  1.00 15.94      A   C
ATOM  1378  CG2 ILE A 177      29.805  65.149  28.759  1.00 14.07      A   C
ATOM  1379  CG1 ILE A 177      31.113  64.699  26.647  1.00 17.19      A   C
ATOM  1380  CD1 ILE A 177      29.880  64.597  25.748  1.00 18.12      A   C
ATOM  1381  C   ILE A 177      31.896  63.970  30.334  1.00 14.25      A   C
ATOM  1382  O   ILE A 177      31.499  62.833  30.609  1.00 15.75      A   O
ATOM  1383  N   ILE A 178      32.108  64.900  31.253  1.00 14.90      A   N
ATOM  1384  CA  ILE A 178      31.841  64.618  32.647  1.00 12.36      A   C
ATOM  1385  CB  ILE A 178      32.770  65.419  33.573  1.00 14.08      A   C
ATOM  1386  CG2 ILE A 178      32.465  65.085  35.026  1.00 10.97      A   C
ATOM  1387  CG1 ILE A 178      34.229  65.095  33.248  1.00 13.91      A   C
ATOM  1388  CD1 ILE A 178      35.235  65.846  34.106  1.00 13.08      A   C
ATOM  1389  C   ILE A 178      30.396  64.988  32.950  1.00 12.88      A   C
ATOM  1390  O   ILE A 178      29.949  66.103  32.671  1.00 13.50      A   O
ATOM  1391  N   LEU A 179      29.659  64.038  33.506  1.00 12.90      A   N
ATOM  1392  CA  LEU A 179      28.270  64.288  33.867  1.00 14.35      A   C
ATOM  1393  CB  LEU A 179      27.465  62.992  33.717  1.00 14.31      A   C
ATOM  1394  CG  LEU A 179      27.542  62.418  32.298  1.00 15.12      A   C
ATOM  1395  CD1 LEU A 179      26.919  61.033  32.251  1.00 20.10      A   C
ATOM  1396  CD2 LEU A 179      26.844  63.361  31.336  1.00 20.25      A   C
ATOM  1397  C   LEU A 179      28.320  64.760  35.319  1.00 13.67      A   C
ATOM  1398  O   LEU A 179      27.829  64.085  36.224  1.00 15.54      A   O
ATOM  1399  N   GLY A 180      28.930  65.931  35.512  1.00 11.65      A   N
ATOM  1400  CA  GLY A 180      29.117  66.517  36.834  1.00 12.90      A   C
ATOM  1401  C   GLY A 180      27.910  67.040  37.593  1.00 10.74      A   C
ATOM  1402  O   GLY A 180      27.955  68.116  38.191  1.00 12.43      A   O
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Figure 7Z

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ATOM  1403 N   CYS A 181    26.835  66.267  37.589  1.00 11.19    A   N
ATOM  1404 CA  CYS A 181    25.608  66.640  38.287  1.00 12.85    A   C
ATOM  1405 CB  CYS A 181    24.832  67.662  37.455  1.00 10.63    A   C
ATOM  1406 SG  CYS A 181    23.232  68.156  38.139  1.00 12.80    A   S
ATOM  1407 C   CYS A 181    24.769  65.379  38.482  1.00 10.40    A   C
ATOM  1408 O   CYS A 181    24.655  64.567  37.565  1.00 12.33    A   O
ATOM  1409 N   THR A 182    24.195  65.218  39.673  1.00 11.84    A   N
ATOM  1410 CA  THR A 182    23.374  64.050  39.993  1.00 10.35    A   C
ATOM  1411 CB  THR A 182    22.661  64.207  41.363  1.00 10.67    A   C
ATOM  1412 OG1 THR A 182    21.912  65.435  41.381  1.00  8.58    A   O
ATOM  1413 CG2 THR A 182    23.672  64.197  42.500  1.00  7.64    A   C
ATOM  1414 C   THR A 182    22.283  63.760  38.966  1.00 11.06    A   C
ATOM  1415 O   THR A 182    21.936  62.610  38.733  1.00 10.76    A   O
ATOM  1416 N   HIS A 183    21.739  64.810  38.364  1.00  9.82    A   N
ATOM  1417 CA  HIS A 183    20.649  64.666  37.400  1.00 12.23    A   C
ATOM  1418 CB  HIS A 183    19.884  65.990  37.276  1.00 10.20    A   C
ATOM  1419 CG  HIS A 183    19.136  66.386  38.510  1.00 10.97    A   C
ATOM  1420 CD2 HIS A 183    17.905  66.930  38.668  1.00  7.50    A   C
ATOM  1421 ND1 HIS A 183    19.677  66.290  39.774  1.00 11.77    A   N
ATOM  1422 CE1 HIS A 183    18.812  66.758  40.658  1.00 10.61    A   C
ATOM  1423 NE2 HIS A 183    17.729  67.154  40.012  1.00 10.59    A   N
ATOM  1424 C   HIS A 183    21.020  64.221  35.990  1.00 10.73    A   C
ATOM  1425 O   HIS A 183    20.228  63.569  35.323  1.00 12.38    A   O
ATOM  1426 N   PHE A 184    22.221  64.570  35.545  1.00 12.86    A   N
ATOM  1427 CA  PHE A 184    22.645  64.280  34.180  1.00 12.13    A   C
ATOM  1428 CB  PHE A 184    23.988  64.976  33.925  1.00 11.91    A   C
ATOM  1429 CG  PHE A 184    23.927  66.488  34.096  1.00 11.77    A   C
ATOM  1430 CD1 PHE A 184    25.057  67.276  33.896  1.00 13.67    A   C
ATOM  1431 CD2 PHE A 184    22.739  67.116  34.482  1.00  9.45    A   C
ATOM  1432 CE1 PHE A 184    25.009  68.666  34.081  1.00 11.33    A   C
ATOM  1433 CE2 PHE A 184    22.681  68.502  34.670  1.00 12.83    A   C
ATOM  1434 CZ  PHE A 184    23.819  69.278  34.469  1.00  9.95    A   C
ATOM  1435 C   PHE A 184    22.655  62.833  33.670  1.00 12.53    A   C
ATOM  1436 O   PHE A 184    22.429  62.596  32.481  1.00 14.09    A   O
ATOM  1437 N   PRO A 185    22.902  61.847  34.545  1.00 13.81    A   N
ATOM  1438 CD  PRO A 185    23.442  61.881  35.918  1.00 14.48    A   C
ATOM  1439 CA  PRO A 185    22.893  60.475  34.026  1.00 13.96    A   C
ATOM  1440 CB  PRO A 185    23.165  59.640  35.275  1.00 14.58    A   C
ATOM  1441 CG  PRO A 185    24.112  60.522  36.032  1.00 12.13    A   C
ATOM  1442 C   PRO A 185    21.554  60.121  33.367  1.00 15.04    A   C
ATOM  1443 O   PRO A 185    21.492  59.261  32.489  1.00 13.75    A   O
ATOM  1444 N   LEU A 186    20.485  60.790  33.791  1.00 13.98    A   N
ATOM  1445 CA  LEU A 186    19.156  60.525  33.243  1.00 13.19    A   C
ATOM  1446 CB  LEU A 186    18.080  61.193  34.108  1.00 13.71    A   C
ATOM  1447 CG  LEU A 186    17.634  60.379  35.334  1.00 15.55    A   C
ATOM  1448 CD1 LEU A 186    18.802  60.174  36.288  1.00 18.92    A   C
ATOM  1449 CD2 LEU A 186    16.493  61.099  36.027  1.00 14.26    A   C
ATOM  1450 C   LEU A 186    18.982  60.931  31.778  1.00 14.41    A   C
ATOM  1451 O   LEU A 186    18.010  60.533  31.137  1.00 14.59    A   O
ATOM  1452 N   ILE A 187    19.905  61.734  31.255  1.00 14.30    A   N
ATOM  1453 CA  ILE A 187    19.854  62.140  29.849  1.00 14.33    A   C
ATOM  1454 CB  ILE A 187    19.485  63.633  29.667  1.00 13.17    A   C
ATOM  1455 CG2 ILE A 187    18.052  63.871  30.096  1.00 11.03    A   C
ATOM  1456 CG1 ILE A 187    20.446  64.523  30.453  1.00 12.17    A   C
ATOM  1457 CD1 ILE A 187    20.256  66.011  30.170  1.00 14.07    A   C
ATOM  1458 C   ILE A 187    21.197  61.890  29.168  1.00 14.64    A   C
ATOM  1459 O   ILE A 187    21.487  62.447  28.108  1.00 13.68    A   O
ATOM  1460 N   ALA A 188    22.008  61.035  29.781  1.00 15.37    A   N
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Figure 7AA

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ATOM  1461  CA  ALA A 188     23.322  60.707  29.243  1.00 16.86      A   C
ATOM  1462  CB  ALA A 188     23.965  59.607  30.075  1.00 15.17      A   C
ATOM  1463  C   ALA A 188     23.244  60.280  27.776  1.00 17.17      A   C
ATOM  1464  O   ALA A 188     23.979  60.797  26.938  1.00 15.74      A   O
ATOM  1465  N   GLN A 189     22.353  59.340  27.470  1.00 17.32      A   N
ATOM  1466  CA  GLN A 189     22.203  58.857  26.101  1.00 18.82      A   C
ATOM  1467  CB  GLN A 189     21.162  57.741  26.050  1.00 23.61      A   C
ATOM  1468  CG  GLN A 189     21.199  56.919  24.774  1.00 30.80      A   C
ATOM  1469  CD  GLN A 189     22.592  56.391  24.458  1.00 36.03      A   C
ATOM  1470  OE1 GLN A 189     23.321  55.942  25.347  1.00 36.39      A   O
ATOM  1471  NE2 GLN A 189     22.965  56.435  23.184  1.00 38.93      A   N
ATOM  1472  C   GLN A 189     21.794  59.995  25.169  1.00 17.49      A   C
ATOM  1473  O   GLN A 189     22.280  60.092  24.041  1.00 17.22      A   O
ATOM  1474  N   LYS A 190     20.894  60.851  25.639  1.00 17.64      A   N
ATOM  1475  CA  LYS A 190     20.449  61.986  24.841  1.00 16.93      A   C
ATOM  1476  CB  LYS A 190     19.338  62.750  25.565  1.00 17.51      A   C
ATOM  1477  CG  LYS A 190     17.998  62.038  25.578  1.00 21.98      A   C
ATOM  1478  CD  LYS A 190     17.462  61.852  24.166  1.00 25.56      A   C
ATOM  1479  CE  LYS A 190     16.064  61.256  24.188  1.00 30.02      A   C
ATOM  1480  NZ  LYS A 190     15.428  61.242  22.839  1.00 32.59      A   N
ATOM  1481  C   LYS A 190     21.624  62.919  24.572  1.00 17.12      A   C
ATOM  1482  O   LYS A 190     21.755  63.468  23.481  1.00 19.51      A   O
ATOM  1483  N   ILE A 191     22.483  63.097  25.570  1.00 15.92      A   N
ATOM  1484  CA  ILE A 191     23.643  63.963  25.413  1.00 15.53      A   C
ATOM  1485  CB  ILE A 191     24.348  64.194  26.769  1.00 16.74      A   C
ATOM  1486  CG2 ILE A 191     25.698  64.877  26.558  1.00 17.54      A   C
ATOM  1487  CG1 ILE A 191     23.447  65.048  27.668  1.00 16.67      A   C
ATOM  1488  CD1 ILE A 191     24.051  65.372  29.014  1.00 17.95      A   C
ATOM  1489  C   ILE A 191     24.615  63.350  24.413  1.00 17.26      A   C
ATOM  1490  O   ILE A 191     25.099  64.027  23.508  1.00 16.51      A   O
ATOM  1491  N   GLU A 192     24.892  62.062  24.566  1.00 17.44      A   N
ATOM  1492  CA  GLU A 192     25.792  61.387  23.643  1.00 18.42      A   C
ATOM  1493  CB  GLU A 192     25.937  59.909  24.007  1.00 20.11      A   C
ATOM  1494  CG  GLU A 192     26.885  59.159  23.085  1.00 26.76      A   C
ATOM  1495  CD  GLU A 192     26.872  57.665  23.322  1.00 32.66      A   C
ATOM  1496  OE1 GLU A 192     25.884  57.005  22.936  1.00 37.07      A   O
ATOM  1497  OE2 GLU A 192     27.846  57.152  23.906  1.00 37.14      A   O
ATOM  1498  C   GLU A 192     25.209  61.499  22.241  1.00 17.46      A   C
ATOM  1499  O   GLU A 192     25.912  61.804  21.283  1.00 15.49      A   O
ATOM  1500  N   GLY A 193     23.910  61.249  22.136  1.00 19.60      A   N
ATOM  1501  CA  GLY A 193     23.247  61.319  20.851  1.00 18.22      A   C
ATOM  1502  C   GLY A 193     23.344  62.683  20.199  1.00 20.98      A   C
ATOM  1503  O   GLY A 193     23.518  62.781  18.983  1.00 19.02      A   O
ATOM  1504  N   TYR A 194     23.230  63.742  20.997  1.00 19.99      A   N
ATOM  1505  CA  TYR A 194     23.302  65.087  20.450  1.00 19.30      A   C
ATOM  1506  CB  TYR A 194     23.081  66.136  21.545  1.00 21.79      A   C
ATOM  1507  CG  TYR A 194     23.038  67.544  20.997  1.00 22.73      A   C
ATOM  1508  CD1 TYR A 194     21.822  68.170  20.713  1.00 25.33      A   C
ATOM  1509  CE1 TYR A 194     21.784  69.442  20.133  1.00 26.15      A   C
ATOM  1510  CD2 TYR A 194     24.216  68.226  20.692  1.00 24.23      A   C
ATOM  1511  CE2 TYR A 194     24.190  69.493  20.109  1.00 23.26      A   C
ATOM  1512  CZ  TYR A 194     22.973  70.092  19.830  1.00 25.26      A   C
ATOM  1513  OH  TYR A 194     22.941  71.327  19.222  1.00 28.86      A   O
ATOM  1514  C   TYR A 194     24.660  65.313  19.788  1.00 20.71      A   C
ATOM  1515  O   TYR A 194     24.738  65.782  18.653  1.00 18.94      A   O
ATOM  1516  N   PHE A 195     25.732  64.980  20.496  1.00 19.26      A   N
ATOM  1517  CA  PHE A 195     27.062  65.169  19.942  1.00 21.38      A   C
ATOM  1518  CB  PHE A 195     28.126  64.952  21.020  1.00 20.73      A   C
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Figure 7BB

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ATOM  1519  CG  PHE A 195     28.251  66.103  21.971  1.00 20.61      A   C
ATOM  1520  CD1 PHE A 195     27.488  66.158  23.131  1.00 19.23      A   C
ATOM  1521  CD2 PHE A 195     29.097  67.165  21.673  1.00 21.43      A   C
ATOM  1522  CE1 PHE A 195     27.565  67.263  23.986  1.00 20.28      A   C
ATOM  1523  CE2 PHE A 195     29.183  68.273  22.515  1.00 18.52      A   C
ATOM  1524  CZ  PHE A 195     28.416  68.323  23.673  1.00 19.62      A   C
ATOM  1525  C   PHE A 195     27.352  64.290  18.730  1.00 21.31      A   C
ATOM  1526  O   PHE A 195     28.045  64.713  17.806  1.00 21.45      A   O
ATOM  1527  N   MET A 196     26.822  63.072  18.720  1.00 22.22      A   N
ATOM  1528  CA  MET A 196     27.059  62.190  17.584  1.00 24.31      A   C
ATOM  1529  CB  MET A 196     26.655  60.749  17.915  1.00 25.67      A   C
ATOM  1530  CG  MET A 196     27.528  60.084  18.971  1.00 26.49      A   C
ATOM  1531  SD  MET A 196     29.295  60.205  18.575  1.00 30.70      A   S
ATOM  1532  CE  MET A 196     29.481  58.865  17.401  1.00 31.02      A   C
ATOM  1533  C   MET A 196     26.293  62.667  16.354  1.00 25.42      A   C
ATOM  1534  O   MET A 196     26.734  62.451  15.227  1.00 23.73      A   O
ATOM  1535  N   GLY A 197     25.157  63.328  16.571  1.00 25.90      A   N
ATOM  1536  CA  GLY A 197     24.361  63.805  15.451  1.00 26.44      A   C
ATOM  1537  C   GLY A 197     24.566  65.258  15.054  1.00 29.06      A   C
ATOM  1538  O   GLY A 197     24.129  65.681  13.981  1.00 30.51      A   O
ATOM  1539  N   HIS A 198     25.233  66.030  15.903  1.00 27.75      A   N
ATOM  1540  CA  HIS A 198     25.456  67.441  15.612  1.00 28.55      A   C
ATOM  1541  CB  HIS A 198     24.824  68.293  16.705  1.00 28.88      A   C
ATOM  1542  CG  HIS A 198     23.330  68.234  16.718  1.00 26.12      A   C
ATOM  1543  CD2 HIS A 198     22.470  67.535  17.495  1.00 26.28      A   C
ATOM  1544  ND1 HIS A 198     22.553  68.943  15.828  1.00 27.58      A   N
ATOM  1545  CE1 HIS A 198     21.277  68.687  16.060  1.00 27.01      A   C
ATOM  1546  NE2 HIS A 198     21.200  67.835  17.066  1.00 26.83      A   N
ATOM  1547  C   HIS A 198     26.923  67.792  15.457  1.00 30.79      A   C
ATOM  1548  O   HIS A 198     27.270  68.941  15.180  1.00 32.29      A   O
ATOM  1549  N   PHE A 199     27.785  66.800  15.644  1.00 30.80      A   N
ATOM  1550  CA  PHE A 199     29.220  66.999  15.498  1.00 33.66      A   C
ATOM  1551  CB  PHE A 199     29.906  67.052  16.866  1.00 35.46      A   C
ATOM  1552  CG  PHE A 199     29.565  68.275  17.676  1.00 39.04      A   C
ATOM  1553  CD1 PHE A 199     28.281  68.463  18.182  1.00 39.24      A   C
ATOM  1554  CD2 PHE A 199     30.537  69.237  17.945  1.00 40.88      A   C
ATOM  1555  CE1 PHE A 199     27.968  69.591  18.944  1.00 40.57      A   C
ATOM  1556  CE2 PHE A 199     30.236  70.370  18.707  1.00 42.99      A   C
ATOM  1557  CZ  PHE A 199     28.948  70.547  19.207  1.00 40.25      A   C
ATOM  1558  C   PHE A 199     29.790  65.855  14.673  1.00 32.87      A   C
ATOM  1559  O   PHE A 199     29.170  64.798  14.547  1.00 32.00      A   O
ATOM  1560  N   ALA A 200     30.972  66.064  14.108  1.00 34.09      A   N
ATOM  1561  CA  ALA A 200     31.605  65.040  13.288  1.00 34.34      A   C
ATOM  1562  CB  ALA A 200     32.381  65.690  12.154  1.00 35.22      A   C
ATOM  1563  C   ALA A 200     32.532  64.168  14.119  1.00 34.93      A   C
ATOM  1564  O   ALA A 200     33.704  63.996  13.782  1.00 35.08      A   O
ATOM  1565  N   LEU A 201     32.012  63.618  15.209  1.00 34.85      A   N
ATOM  1566  CA  LEU A 201     32.821  62.765  16.067  1.00 34.78      A   C
ATOM  1567  CB  LEU A 201     32.210  62.690  17.472  1.00 35.79      A   C
ATOM  1568  CG  LEU A 201     32.120  64.015  18.231  1.00 35.31      A   C
ATOM  1569  CD1 LEU A 201     31.513  63.760  19.603  1.00 35.13      A   C
ATOM  1570  CD2 LEU A 201     33.498  64.641  18.365  1.00 35.35      A   C
ATOM  1571  C   LEU A 201     32.906  61.366  15.462  1.00 34.07      A   C
ATOM  1572  O   LEU A 201     31.887  60.773  15.104  1.00 35.38      A   O
ATOM  1573  N   PRO A 202     34.128  60.817  15.344  1.00 33.66      A   N
ATOM  1574  CD  PRO A 202     35.409  61.457  15.698  1.00 32.39      A   C
ATOM  1575  CA  PRO A 202     34.353  59.475  14.779  1.00 32.85      A   C
ATOM  1576  CB  PRO A 202     35.872  59.404  14.655  1.00 33.65      A   C
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Figure 7CC

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ATOM  1577  CG  PRO A 202      36.343  60.272  15.793  1.00 34.48      A   C
ATOM  1578  C   PRO A 202      33.790  58.355  15.649  1.00 33.17      A   C
ATOM  1579  O   PRO A 202      33.402  57.297  15.151  1.00 30.49      A   O
ATOM  1580  N   THR A 203      33.773  58.599  16.956  1.00 31.52      A   N
ATOM  1581  CA  THR A 203      33.248  57.634  17.919  1.00 31.65      A   C
ATOM  1582  CB  THR A 203      34.338  56.676  18.426  1.00 32.68      A   C
ATOM  1583  OG1 THR A 203      35.425  57.424  18.979  1.00 35.29      A   O
ATOM  1584  CG2 THR A 203      34.828  55.781  17.302  1.00 37.32      A   C
ATOM  1585  C   THR A 203      32.688  58.386  19.117  1.00 30.86      A   C
ATOM  1586  O   THR A 203      33.168  59.451  19.461  1.00 27.18      A   O
ATOM  1587  N   PRO A 204      31.671  57.817  19.775  1.00 29.89      A   N
ATOM  1588  CD  PRO A 204      31.126  56.473  19.492  1.00 29.77      A   C
ATOM  1589  CA  PRO A 204      31.061  58.463  20.945  1.00 28.24      A   C
ATOM  1590  CB  PRO A 204      30.047  57.449  21.462  1.00 29.94      A   C
ATOM  1591  CG  PRO A 204      30.111  56.276  20.568  1.00 30.77      A   C
ATOM  1592  C   PRO A 204      32.096  58.803  22.007  1.00 25.79      A   C
ATOM  1593  O   PRO A 204      33.032  58.041  22.269  1.00 25.89      A   O
ATOM  1594  N   PRO A 205      31.961  59.981  22.626  1.00 23.44      A   N
ATOM  1595  CD  PRO A 205      30.990  61.063  22.358  1.00 24.13      A   C
ATOM  1596  CA  PRO A 205      32.915  60.378  23.670  1.00 22.08      A   C
ATOM  1597  CB  PRO A 205      32.600  61.852  23.873  1.00 24.52      A   C
ATOM  1598  CG  PRO A 205      31.125  61.932  23.587  1.00 24.69      A   C
ATOM  1599  C   PRO A 205      32.705  59.546  24.927  1.00 19.36      A   C
ATOM  1600  O   PRO A 205      31.637  58.961  25.125  1.00 18.49      A   O
ATOM  1601  N   LEU A 206      33.722  59.492  25.776  1.00 18.43      A   N
ATOM  1602  CA  LEU A 206      33.626  58.762  27.037  1.00 18.50      A   C
ATOM  1603  CB  LEU A 206      35.018  58.513  27.619  1.00 20.51      A   C
ATOM  1604  CG  LEU A 206      35.095  57.847  28.996  1.00 22.39      A   C
ATOM  1605  CD1 LEU A 206      34.491  56.439  28.946  1.00 22.36      A   C
ATOM  1606  CD2 LEU A 206      36.552  57.791  29.435  1.00 24.60      A   C
ATOM  1607  C   LEU A 206      32.822  59.615  28.017  1.00 18.04      A   C
ATOM  1608  O   LEU A 206      33.163  60.770  28.253  1.00 16.95      A   O
ATOM  1609  N   LEU A 207      31.746  59.049  28.554  1.00 16.00      A   N
ATOM  1610  CA  LEU A 207      30.909  59.748  29.521  1.00 17.26      A   C
ATOM  1611  CB  LEU A 207      29.433  59.412  29.304  1.00 18.06      A   C
ATOM  1612  CG  LEU A 207      28.664  60.071  28.158  1.00 24.42      A   C
ATOM  1613  CD1 LEU A 207      29.448  59.984  26.863  1.00 25.51      A   C
ATOM  1614  CD2 LEU A 207      27.310  59.373  28.012  1.00 24.48      A   C
ATOM  1615  C   LEU A 207      31.318  59.314  30.922  1.00 16.98      A   C
ATOM  1616  O   LEU A 207      31.388  58.120  31.215  1.00 18.46      A   O
ATOM  1617  N   ILE A 208      31.592  60.276  31.792  1.00 13.50      A   N
ATOM  1618  CA  ILE A 208      31.983  59.940  33.150  1.00 14.98      A   C
ATOM  1619  CB  ILE A 208      33.112  60.864  33.659  1.00 16.20      A   C
ATOM  1620  CG2 ILE A 208      33.468  60.509  35.101  1.00 16.97      A   C
ATOM  1621  CG1 ILE A 208      34.345  60.722  32.763  1.00 16.39      A   C
ATOM  1622  CD1 ILE A 208      34.984  59.333  32.784  1.00 17.91      A   C
ATOM  1623  C   ILE A 208      30.771  60.069  34.057  1.00 15.79      A   C
ATOM  1624  O   ILE A 208      30.193  61.150  34.194  1.00 15.47      A   O
ATOM  1625  N   HIS A 209      30.390  58.951  34.669  1.00 15.02      A   N
ATOM  1626  CA  HIS A 209      29.238  58.895  35.567  1.00 14.90      A   C
ATOM  1627  CB  HIS A 209      28.502  57.569  35.333  1.00 17.49      A   C
ATOM  1628  CG  HIS A 209      27.271  57.387  36.169  1.00 19.71      A   C
ATOM  1629  CD2 HIS A 209      27.116  57.192  37.500  1.00 20.19      A   C
ATOM  1630  ND1 HIS A 209      26.004  57.336  35.625  1.00 21.72      A   N
ATOM  1631  CE1 HIS A 209      25.123  57.114  36.584  1.00 17.63      A   C
ATOM  1632  NE2 HIS A 209      25.772  57.023  37.732  1.00 22.48      A   N
ATOM  1633  C   HIS A 209      29.744  59.006  37.011  1.00 13.24      A   C
ATOM  1634  O   HIS A 209      30.546  58.191  37.458  1.00 13.01      A   O
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Figure 7DD

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ATOM  1635  N  SER A 210    29.275  60.018  37.734  1.00 12.05    A   N
ATOM  1636  CA  SER A 210    29.709  60.238  39.109  1.00 11.23    A   C
ATOM  1637  CB  SER A 210    28.977  61.442  39.701  1.00 11.83    A   C
ATOM  1638  OG  SER A 210    29.140  62.587  38.881  1.00 12.14    A   O
ATOM  1639  C  SER A 210    29.529  59.031  40.032  1.00 12.17    A   C
ATOM  1640  O  SER A 210    30.370  58.774  40.890  1.00 11.45    A   O
ATOM  1641  N  GLY A 211    28.432  58.303  39.861  1.00 13.88    A   N
ATOM  1642  CA  GLY A 211    28.178  57.142  40.698  1.00 15.08    A   C
ATOM  1643  C  GLY A 211    29.147  56.004  40.446  1.00 16.38    A   C
ATOM  1644  O  GLY A 211    29.744  55.461  41.378  1.00 15.04    A   O
ATOM  1645  N  ASP A 212    29.311  55.630  39.183  1.00 15.98    A   N
ATOM  1646  CA  ASP A 212    30.231  54.552  38.860  1.00 16.82    A   C
ATOM  1647  CB  ASP A 212    30.208  54.264  37.365  1.00 19.63    A   C
ATOM  1648  CG  ASP A 212    28.847  53.798  36.895  1.00 23.61    A   C
ATOM  1649  OD1 ASP A 212    28.145  53.131  37.692  1.00 25.34    A   O
ATOM  1650  OD2 ASP A 212    28.486  54.086  35.738  1.00 21.50    A   O
ATOM  1651  C  ASP A 212    31.638  54.917  39.303  1.00 16.04    A   C
ATOM  1652  O  ASP A 212    32.375  54.073  39.807  1.00 15.40    A   O
ATOM  1653  N  ALA A 213    31.994  56.185  39.135  1.00 12.67    A   N
ATOM  1654  CA  ALA A 213    33.317  56.667  39.517  1.00 14.11    A   C
ATOM  1655  CB  ALA A 213    33.493  58.126  39.076  1.00 11.29    A   C
ATOM  1656  C  ALA A 213    33.560  56.540  41.022  1.00 12.53    A   C
ATOM  1657  O  ALA A 213    34.607  56.049  41.452  1.00 13.00    A   O
ATOM  1658  N  ILE A 214    32.603  56.973  41.834  1.00 13.61    A   N
ATOM  1659  CA  ILE A 214    32.808  56.875  43.271  1.00 11.94    A   C
ATOM  1660  CB  ILE A 214    31.748  57.701  44.065  1.00 12.63    A   C
ATOM  1661  CG2 ILE A 214    30.367  57.085  43.938  1.00 15.04    A   C
ATOM  1662  CG1 ILE A 214    32.174  57.795  45.530  1.00 12.30    A   C
ATOM  1663  CD1 ILE A 214    31.429  58.832  46.317  1.00 11.04    A   C
ATOM  1664  C  ILE A 214    32.855  55.405  43.719  1.00 13.71    A   C
ATOM  1665  O  ILE A 214    33.595  55.061  44.643  1.00 12.81    A   O
ATOM  1666  N  VAL A 215    32.096  54.538  43.053  1.00 13.33    A   N
ATOM  1667  CA  VAL A 215    32.118  53.109  43.387  1.00 13.18    A   C
ATOM  1668  CB  VAL A 215    31.165  52.293  42.474  1.00 13.68    A   C
ATOM  1669  CG1 VAL A 215    31.481  50.792  42.579  1.00 14.80    A   C
ATOM  1670  CG2 VAL A 215    29.707  52.537  42.876  1.00 10.93    A   C
ATOM  1671  C  VAL A 215    33.550  52.599  43.190  1.00 15.07    A   C
ATOM  1672  O  VAL A 215    34.115  51.933  44.065  1.00 12.73    A   O
ATOM  1673  N  GLU A 216    34.136  52.924  42.039  1.00 13.86    A   N
ATOM  1674  CA  GLU A 216    35.503  52.511  41.738  1.00 17.89    A   C
ATOM  1675  CB  GLU A 216    35.973  53.120  40.414  1.00 21.27    A   C
ATOM  1676  CG  GLU A 216    35.112  52.807  39.204  1.00 27.92    A   C
ATOM  1677  CD  GLU A 216    35.637  53.492  37.941  1.00 34.02    A   C
ATOM  1678  OE1 GLU A 216    36.824  53.286  37.609  1.00 31.93    A   O
ATOM  1679  OE2 GLU A 216    34.868  54.236  37.285  1.00 35.33    A   O
ATOM  1680  C  GLU A 216    36.447  52.971  42.846  1.00 17.32    A   C
ATOM  1681  O  GLU A 216    37.245  52.188  43.363  1.00 16.80    A   O
ATOM  1682  N  TYR A 217    36.352  54.248  43.204  1.00 16.20    A   N
ATOM  1683  CA  TYR A 217    37.200  54.818  44.244  1.00 16.23    A   C
ATOM  1684  CB  TYR A 217    36.900  56.308  44.432  1.00 14.73    A   C
ATOM  1685  CG  TYR A 217    37.693  56.942  45.557  1.00 17.55    A   C
ATOM  1686  CD1 TYR A 217    39.053  57.202  45.418  1.00 18.17    A   C
ATOM  1687  CE1 TYR A 217    39.797  57.738  46.475  1.00 18.51    A   C
ATOM  1688  CD2 TYR A 217    37.089  57.234  46.780  1.00 16.61    A   C
ATOM  1689  CE2 TYR A 217    37.815  57.765  47.836  1.00 17.74    A   C
ATOM  1690  CZ  TYR A 217    39.168  58.014  47.680  1.00 19.47    A   C
ATOM  1691  OH  TYR A 217    39.891  58.526  48.735  1.00 18.42    A   O
ATOM  1692  C  TYR A 217    37.041  54.116  45.584  1.00 16.31    A   C
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Figure 7EE

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ATOM  1693  O   TYR A 217     38.028  53.715  46.199  1.00 16.78    A   O
ATOM  1694  N   LEU A 218     35.798  53.995  46.045  1.00 15.56    A   N
ATOM  1695  CA  LEU A 218     35.509  53.353  47.324  1.00 18.16    A   C
ATOM  1696  CB  LEU A 218     33.993  53.344  47.575  1.00 15.21    A   C
ATOM  1697  CG  LEU A 218     33.321  54.705  47.799  1.00 15.27    A   C
ATOM  1698  CD1 LEU A 218     31.798  54.546  47.756  1.00 14.34    A   C
ATOM  1699  CD2 LEU A 218     33.775  55.294  49.129  1.00 13.25    A   C
ATOM  1700  C   LEU A 218     36.058  51.926  47.402  1.00 18.45    A   C
ATOM  1701  O   LEU A 218     36.648  51.531  48.409  1.00 18.06    A   O
ATOM  1702  N   GLN A 219     35.871  51.150  46.341  1.00 17.77    A   N
ATOM  1703  CA  GLN A 219     36.367  49.778  46.335  1.00 19.66    A   C
ATOM  1704  CB  GLN A 219     36.042  49.097  45.005  1.00 18.42    A   C
ATOM  1705  CG  GLN A 219     34.577  49.147  44.645  1.00 17.80    A   C
ATOM  1706  CD  GLN A 219     34.282  48.496  43.318  1.00 17.89    A   C
ATOM  1707  OE1 GLN A 219     35.071  48.596  42.372  1.00 18.96    A   O
ATOM  1708  NE2 GLN A 219     33.134  47.837  43.228  1.00 13.87    A   N
ATOM  1709  C   GLN A 219     37.876  49.740  46.567  1.00 19.63    A   C
ATOM  1710  O   GLN A 219     38.368  48.964  47.380  1.00 19.95    A   O
ATOM  1711  N   GLN A 220     38.605  50.593  45.859  1.00 21.16    A   N
ATOM  1712  CA  GLN A 220     40.057  50.621  45.992  1.00 24.11    A   C
ATOM  1713  CB  GLN A 220     40.681  51.372  44.811  1.00 25.85    A   C
ATOM  1714  CG  GLN A 220     42.197  51.445  44.885  1.00 34.94    A   C
ATOM  1715  CD  GLN A 220     42.830  51.975  43.615  1.00 40.03    A   C
ATOM  1716  OE1 GLN A 220     44.050  52.152  43.548  1.00 44.37    A   O
ATOM  1717  NE2 GLN A 220     42.010  52.227  42.598  1.00 41.95    A   N
ATOM  1718  C   GLN A 220     40.534  51.242  47.304  1.00 22.63    A   C
ATOM  1719  O   GLN A 220     41.275  50.617  48.062  1.00 21.00    A   O
ATOM  1720  N   LYS A 221     40.104  52.472  47.564  1.00 21.71    A   N
ATOM  1721  CA  LYS A 221     40.503  53.194  48.770  1.00 22.37    A   C
ATOM  1722  CB  LYS A 221     39.830  54.570  48.795  1.00 21.53    A   C
ATOM  1723  CG  LYS A 221     39.984  55.325  50.111  1.00 25.31    A   C
ATOM  1724  CD  LYS A 221     41.443  55.615  50.439  1.00 26.19    A   C
ATOM  1725  CE  LYS A 221     41.579  56.244  51.818  1.00 29.00    A   C
ATOM  1726  NZ  LYS A 221     42.999  56.511  52.159  1.00 29.71    A   N
ATOM  1727  C   LYS A 221     40.221  52.464  50.084  1.00 22.42    A   C
ATOM  1728  O   LYS A 221     41.090  52.376  50.953  1.00 21.37    A   O
ATOM  1729  N   TYR A 222     39.005  51.950  50.229  1.00 20.94    A   N
ATOM  1730  CA  TYR A 222     38.616  51.250  51.442  1.00 21.75    A   C
ATOM  1731  CB  TYR A 222     37.251  51.762  51.903  1.00 22.02    A   C
ATOM  1732  CG  TYR A 222     37.277  53.247  52.204  1.00 20.42    A   C
ATOM  1733  CD1 TYR A 222     36.737  54.178  51.314  1.00 18.91    A   C
ATOM  1734  CE1 TYR A 222     36.866  55.549  51.545  1.00 20.88    A   C
ATOM  1735  CD2 TYR A 222     37.938  53.725  53.336  1.00 21.77    A   C
ATOM  1736  CE2 TYR A 222     38.074  55.080  53.577  1.00 19.97    A   C
ATOM  1737  CZ  TYR A 222     37.540  55.988  52.679  1.00 20.71    A   C
ATOM  1738  OH  TYR A 222     37.705  57.330  52.909  1.00 16.95    A   O
ATOM  1739  C   TYR A 222     38.637  49.731  51.350  1.00 21.67    A   C
ATOM  1740  O   TYR A 222     38.112  49.040  52.226  1.00 20.83    A   O
ATOM  1741  N   ALA A 223     39.264  49.219  50.292  1.00 21.20    A   N
ATOM  1742  CA  ALA A 223     39.408  47.774  50.077  1.00 22.92    A   C
ATOM  1743  CB  ALA A 223     40.466  47.204  50.984  1.00 23.23    A   C
ATOM  1744  C   ALA A 223     38.105  47.055  50.330  1.00 23.19    A   C
ATOM  1745  O   ALA A 223     38.024  46.162  51.180  1.00 20.95    A   O
ATOM  1746  N   LEU A 224     37.088  47.426  49.565  1.00 25.19    A   N
ATOM  1747  CA  LEU A 224     35.759  46.839  49.692  1.00 24.53    A   C
ATOM  1748  CB  LEU A 224     34.703  47.937  49.609  1.00 22.99    A   C
ATOM  1749  CG  LEU A 224     34.869  49.090  50.607  1.00 21.68    A   C
ATOM  1750  CD1 LEU A 224     33.731  50.099  50.443  1.00 22.66    A   C
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Figure 7FF

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ATOM  1751 CD2 LEU A 224     34.875 48.531 52.022 1.00 23.83    A   C
ATOM  1752 C   LEU A 224     35.576 45.852 48.551 1.00 24.10    A   C
ATOM  1753 O   LEU A 224     35.569 46.259 47.400 1.00 22.11    A   O
ATOM  1754 N   LYS A 225     35.368 44.572 48.866 1.00 26.47    A   N
ATOM  1755 CA  LYS A 225     35.212 43.532 47.846 1.00 25.75    A   C
ATOM  1756 CB  LYS A 225     35.880 42.233 48.331 1.00 26.74    A   C
ATOM  1757 CG  LYS A 225     37.358 42.380 48.669 1.00 28.32    A   C
ATOM  1758 CD  LYS A 225     38.185 42.652 47.421 1.00 31.42    A   C
ATOM  1759 CE  LYS A 225     38.157 41.461 46.478 1.00 32.69    A   C
ATOM  1760 NZ  LYS A 225     39.003 41.698 45.284 1.00 34.46    A   N
ATOM  1761 C   LYS A 225     33.803 43.213 47.340 1.00 24.95    A   C
ATOM  1762 O   LYS A 225     33.568 42.125 46.819 1.00 29.54    A   O
ATOM  1763 N   ASN A 226     32.870 44.143 47.489 1.00 23.13    A   N
ATOM  1764 CA  ASN A 226     31.498 43.938 47.019 1.00 20.01    A   C
ATOM  1765 CB  ASN A 226     31.469 43.729 45.500 1.00 19.42    A   C
ATOM  1766 CG  ASN A 226     32.287 44.755 44.751 1.00 23.12    A   C
ATOM  1767 OD1 ASN A 226     33.342 44.439 44.190 1.00 20.38    A   O
ATOM  1768 ND2 ASN A 226     31.814 45.995 44.743 1.00 16.65    A   N
ATOM  1769 C   ASN A 226     30.800 42.740 47.662 1.00 21.21    A   C
ATOM  1770 O   ASN A 226     30.086 41.999 46.981 1.00 18.29    A   O
ATOM  1771 N   ASN A 227     30.984 42.551 48.963 1.00 22.29    A   N
ATOM  1772 CA  ASN A 227     30.362 41.421 49.641 1.00 22.96    A   C
ATOM  1773 CB  ASN A 227     31.438 40.462 50.163 1.00 22.46    A   C
ATOM  1774 CG  ASN A 227     32.503 41.165 50.982 1.00 21.07    A   C
ATOM  1775 OD1 ASN A 227     32.223 42.137 51.679 1.00 19.99    A   O
ATOM  1776 ND2 ASN A 227     33.733 40.659 50.916 1.00 19.44    A   N
ATOM  1777 C   ASN A 227     29.428 41.805 50.783 1.00 24.57    A   C
ATOM  1778 O   ASN A 227     29.198 41.005 51.690 1.00 21.91    A   O
ATOM  1779 N   ALA A 228     28.891 43.021 50.741 1.00 23.23    A   N
ATOM  1780 CA  ALA A 228     27.969 43.481 51.776 1.00 26.14    A   C
ATOM  1781 CB  ALA A 228     27.806 45.001 51.699 1.00 22.82    A   C
ATOM  1782 C   ALA A 228     26.611 42.793 51.596 1.00 26.93    A   C
ATOM  1783 O   ALA A 228     26.405 42.077 50.619 1.00 26.75    A   O
ATOM  1784 N   CYS A 229     25.698 43.016 52.541 1.00 29.94    A   N
ATOM  1785 CA  CYS A 229     24.359 42.425 52.508 1.00 34.05    A   C
ATOM  1786 CB  CYS A 229     23.438 43.143 53.508 1.00 36.45    A   C
ATOM  1787 SG  CYS A 229     23.886 42.897 55.243 1.00 48.21    A   S
ATOM  1788 C   CYS A 229     23.730 42.476 51.124 1.00 35.31    A   C
ATOM  1789 O   CYS A 229     23.882 43.451 50.399 1.00 35.27    A   O
ATOM  1790 N   THR A 230     23.030 41.412 50.757 1.00 38.04    A   N
ATOM  1791 CA  THR A 230     22.378 41.380 49.466 1.00 40.97    A   C
ATOM  1792 CB  THR A 230     21.965 39.958 49.076 1.00 42.40    A   C
ATOM  1793 OG1 THR A 230     21.273 39.335 50.163 1.00 45.09    A   O
ATOM  1794 CG2 THR A 230     23.190 39.148 48.730 1.00 43.15    A   C
ATOM  1795 C   THR A 230     21.150 42.269 49.476 1.00 41.97    A   C
ATOM  1796 O   THR A 230     20.887 42.971 48.493 1.00 42.37    A   O
ATOM  1797 N   PHE A 231     20.376 42.232 50.552 1.00 42.74    A   N
ATOM  1798 CA  PHE A 231     19.230 43.108 50.576 1.00 43.96    A   C
ATOM  1799 CB  PHE A 231     17.938 42.321 50.366 1.00 49.35    A   C
ATOM  1800 CG  PHE A 231     17.721 41.990 48.907 1.00 55.66    A   C
ATOM  1801 CD1 PHE A 231     18.494 41.004 48.306 1.00 58.70    A   C
ATOM  1802 CD2 PHE A 231     16.903 42.785 48.088 1.00 58.59    A   C
ATOM  1803 CE1 PHE A 231     18.483 40.801 46.922 1.00 60.69    A   C
ATOM  1804 CE2 PHE A 231     16.879 42.597 46.701 1.00 60.58    A   C
ATOM  1805 CZ  PHE A 231     17.668 41.604 46.113 1.00 60.92    A   C
ATOM  1806 C   PHE A 231     19.335 43.912 51.838 1.00 40.83    A   C
ATOM  1807 O   PHE A 231     18.811 43.567 52.886 1.00 42.69    A   O
ATOM  1808 N   PRO A 232     20.153 44.975 51.722 1.00 35.76    A   N
```

Figure 7GG

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ATOM  1809 CD  PRO A 232     20.672  45.196  50.347  1.00 35.27      A   C
ATOM  1810 CA  PRO A 232     20.579  46.028  52.651  1.00 32.93      A   C
ATOM  1811 CB  PRO A 232     21.689  46.764  51.874  1.00 32.41      A   C
ATOM  1812 CG  PRO A 232     21.363  46.497  50.424  1.00 32.47      A   C
ATOM  1813 C   PRO A 232     19.457  46.929  53.137  1.00 29.06      A   C
ATOM  1814 O   PRO A 232     18.456  47.146  52.452  1.00 27.86      A   O
ATOM  1815 N   LYS A 233     19.630  47.440  54.346  1.00 27.89      A   N
ATOM  1816 CA  LYS A 233     18.645  48.314  54.943  1.00 25.66      A   C
ATOM  1817 CB  LYS A 233     18.682  48.188  56.464  1.00 29.61      A   C
ATOM  1818 CG  LYS A 233     18.178  46.843  56.973  1.00 34.08      A   C
ATOM  1819 CD  LYS A 233     18.086  46.829  58.491  1.00 40.01      A   C
ATOM  1820 CE  LYS A 233     19.454  46.996  59.139  1.00 41.92      A   C
ATOM  1821 NZ  LYS A 233     19.351  47.038  60.626  1.00 44.78      A   N
ATOM  1822 C   LYS A 233     18.945  49.739  54.524  1.00 23.25      A   C
ATOM  1823 O   LYS A 233     20.042  50.248  54.738  1.00 20.72      A   O
ATOM  1824 N   VAL A 234     17.959  50.374  53.909  1.00 21.94      A   N
ATOM  1825 CA  VAL A 234     18.122  51.742  53.457  1.00 18.96      A   C
ATOM  1826 CB  VAL A 234     18.171  51.809  51.927  1.00 18.07      A   C
ATOM  1827 CG1 VAL A 234     18.407  53.242  51.484  1.00 15.91      A   C
ATOM  1828 CG2 VAL A 234     19.265  50.884  51.403  1.00 19.03      A   C
ATOM  1829 C   VAL A 234     16.982  52.622  53.945  1.00 19.45      A   C
ATOM  1830 O   VAL A 234     15.810  52.291  53.775  1.00 18.84      A   O
ATOM  1831 N   GLU A 235     17.332  53.749  54.550  1.00 18.70      A   N
ATOM  1832 CA  GLU A 235     16.333  54.682  55.044  1.00 19.65      A   C
ATOM  1833 CB  GLU A 235     16.584  55.029  56.513  1.00 20.87      A   C
ATOM  1834 CG  GLU A 235     16.619  53.849  57.461  1.00 24.25      A   C
ATOM  1835 CD  GLU A 235     16.762  54.287  58.908  1.00 26.71      A   C
ATOM  1836 OE1 GLU A 235     16.924  53.412  59.782  1.00 30.95      A   O
ATOM  1837 OE2 GLU A 235     16.710  55.509  59.174  1.00 28.58      A   O
ATOM  1838 C   GLU A 235     16.433  55.957  54.226  1.00 19.63      A   C
ATOM  1839 O   GLU A 235     17.522  56.339  53.793  1.00 19.08      A   O
ATOM  1840 N   PHE A 236     15.295  56.608  54.008  1.00 16.22      A   N
ATOM  1841 CA  PHE A 236     15.281  57.850  53.260  1.00 15.50      A   C
ATOM  1842 CB  PHE A 236     14.454  57.703  51.985  1.00 16.22      A   C
ATOM  1843 CG  PHE A 236     15.028  56.712  51.008  1.00 16.49      A   C
ATOM  1844 CD1 PHE A 236     14.734  55.352  51.117  1.00 14.80      A   C
ATOM  1845 CD2 PHE A 236     15.906  57.131  50.011  1.00 16.20      A   C
ATOM  1846 CE1 PHE A 236     15.311  54.423  50.249  1.00 16.35      A   C
ATOM  1847 CE2 PHE A 236     16.488  56.213  49.140  1.00 16.85      A   C
ATOM  1848 CZ  PHE A 236     16.191  54.857  49.258  1.00 18.08      A   C
ATOM  1849 C   PHE A 236     14.725  58.953  54.150  1.00 17.81      A   C
ATOM  1850 O   PHE A 236     13.669  58.808  54.771  1.00 17.48      A   O
ATOM  1851 N   HIS A 237     15.473  60.043  54.238  1.00 14.01      A   N
ATOM  1852 CA  HIS A 237     15.077  61.178  55.050  1.00 13.85      A   C
ATOM  1853 CB  HIS A 237     15.976  61.261  56.282  1.00 16.76      A   C
ATOM  1854 CG  HIS A 237     15.871  60.068  57.183  1.00 20.30      A   C
ATOM  1855 CD2 HIS A 237     16.529  58.884  57.176  1.00 22.69      A   C
ATOM  1856 ND1 HIS A 237     14.963  59.994  58.216  1.00 21.64      A   N
ATOM  1857 CE1 HIS A 237     15.065  58.816  58.808  1.00 24.58      A   C
ATOM  1858 NE2 HIS A 237     16.008  58.123  58.196  1.00 24.02      A   N
ATOM  1859 C   HIS A 237     15.240  62.421  54.190  1.00 12.98      A   C
ATOM  1860 O   HIS A 237     15.960  62.402  53.199  1.00 14.24      A   O
ATOM  1861 N   ALA A 238     14.573  63.500  54.571  1.00 14.25      A   N
ATOM  1862 CA  ALA A 238     14.656  64.745  53.822  1.00 14.74      A   C
ATOM  1863 CB  ALA A 238     13.867  64.622  52.523  1.00 13.87      A   C
ATOM  1864 C   ALA A 238     14.105  65.889  54.662  1.00 16.80      A   C
ATOM  1865 O   ALA A 238     13.416  65.662  55.659  1.00 13.41      A   O
ATOM  1866 N   SER A 239     14.419  67.118  54.265  1.00 16.83      A   N
```

Figure 7HH

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ATOM  1867 CA  SER A 239     13.934  68.289  54.982  1.00 15.86    A   C
ATOM  1868 CB  SER A 239     14.874  69.472  54.749  1.00 17.78    A   C
ATOM  1869 OG  SER A 239     15.235  69.570  53.382  1.00 15.31    A   O
ATOM  1870 C   SER A 239     12.526  68.628  54.501  1.00 18.27    A   C
ATOM  1871 O   SER A 239     11.851  69.475  55.081  1.00 19.09    A   O
ATOM  1872 N   GLY A 240     12.093  67.950  53.440  1.00 19.12    A   N
ATOM  1873 CA  GLY A 240     10.764  68.172  52.891  1.00 18.85    A   C
ATOM  1874 C   GLY A 240     10.400  67.108  51.872  1.00 20.08    A   C
ATOM  1875 O   GLY A 240     11.262  66.321  51.462  1.00 19.84    A   O
ATOM  1876 N   ASP A 241     9.134  67.065  51.464  1.00 17.58    A   N
ATOM  1877 CA  ASP A 241     8.692  66.077  50.481  1.00 19.46    A   C
ATOM  1878 CB  ASP A 241     9.150  66.501  49.083  1.00 21.27    A   C
ATOM  1879 CG  ASP A 241     8.429  67.738  48.587  1.00 23.85    A   C
ATOM  1880 OD1 ASP A 241     7.247  67.610  48.206  1.00 26.32    A   O
ATOM  1881 OD2 ASP A 241     9.038  68.833  48.591  1.00 21.42    A   O
ATOM  1882 C   ASP A 241     9.257  64.694  50.803  1.00 16.99    A   C
ATOM  1883 O   ASP A 241     9.731  63.987  49.913  1.00 17.49    A   O
ATOM  1884 N   VAL A 242     9.208  64.316  52.076  1.00 15.93    A   N
ATOM  1885 CA  VAL A 242     9.737  63.025  52.516  1.00 14.13    A   C
ATOM  1886 CB  VAL A 242     9.894  62.990  54.052  1.00 17.19    A   C
ATOM  1887 CG1 VAL A 242     10.671  61.740  54.469  1.00 16.23    A   C
ATOM  1888 CG2 VAL A 242     10.612  64.248  54.523  1.00 18.97    A   C
ATOM  1889 C   VAL A 242     8.849  61.864  52.082  1.00 15.60    A   C
ATOM  1890 O   VAL A 242     9.341  60.808  51.660  1.00 12.78    A   O
ATOM  1891 N   ILE A 243     7.540  62.057  52.209  1.00 14.41    A   N
ATOM  1892 CA  ILE A 243     6.577  61.045  51.803  1.00 16.25    A   C
ATOM  1893 CB  ILE A 243     5.125  61.549  52.007  1.00 18.10    A   C
ATOM  1894 CG2 ILE A 243     4.123  60.554  51.414  1.00 20.99    A   C
ATOM  1895 CG1 ILE A 243     4.858  61.747  53.502  1.00 21.18    A   C
ATOM  1896 CD1 ILE A 243     3.485  62.293  53.817  1.00 20.78    A   C
ATOM  1897 C   ILE A 243     6.833  60.787  50.324  1.00 15.05    A   C
ATOM  1898 O   ILE A 243     6.885  59.639  49.878  1.00 16.76    A   O
ATOM  1899 N   TRP A 244     7.005  61.868  49.569  1.00 13.24    A   N
ATOM  1900 CA  TRP A 244     7.270  61.768  48.142  1.00 15.52    A   C
ATOM  1901 CB  TRP A 244     7.343  63.164  47.523  1.00 13.47    A   C
ATOM  1902 CG  TRP A 244     7.510  63.151  46.036  1.00 18.87    A   C
ATOM  1903 CD2 TRP A 244     8.732  63.342  45.312  1.00 17.48    A   C
ATOM  1904 CE2 TRP A 244     8.426  63.232  43.940  1.00 18.22    A   C
ATOM  1905 CE3 TRP A 244     10.057  63.594  45.693  1.00 17.59    A   C
ATOM  1906 CD1 TRP A 244     6.538  62.938  45.099  1.00 18.15    A   C
ATOM  1907 NE1 TRP A 244     7.083  62.988  43.835  1.00 18.29    A   N
ATOM  1908 CZ2 TRP A 244     9.399  63.366  42.943  1.00 20.22    A   C
ATOM  1909 CZ3 TRP A 244     11.024  63.727  44.702  1.00 18.36    A   C
ATOM  1910 CH2 TRP A 244     10.688  63.611  43.342  1.00 18.43    A   C
ATOM  1911 C   TRP A 244     8.590  61.042  47.891  1.00 14.64    A   C
ATOM  1912 O   TRP A 244     8.670  60.149  47.044  1.00 16.51    A   O
ATOM  1913 N   LEU A 245     9.628  61.436  48.623  1.00 13.56    A   N
ATOM  1914 CA  LEU A 245     10.941  60.814  48.459  1.00 12.19    A   C
ATOM  1915 CB  LEU A 245     11.946  61.416  49.444  1.00 11.28    A   C
ATOM  1916 CG  LEU A 245     13.379  60.875  49.342  1.00 11.24    A   C
ATOM  1917 CD1 LEU A 245     13.988  61.289  48.009  1.00 11.74    A   C
ATOM  1918 CD2 LEU A 245     14.223  61.407  50.490  1.00 10.22    A   C
ATOM  1919 C   LEU A 245     10.862  59.301  48.661  1.00 14.05    A   C
ATOM  1920 O   LEU A 245     11.439  58.537  47.884  1.00 12.33    A   O
ATOM  1921 N   GLU A 246     10.144  58.870  49.698  1.00 14.68    A   N
ATOM  1922 CA  GLU A 246     10.000  57.441  49.980  1.00 16.30    A   C
ATOM  1923 CB  GLU A 246     9.198  57.213  51.267  1.00 16.70    A   C
ATOM  1924 CG  GLU A 246     9.938  57.637  52.521  1.00 23.08    A   C
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Figure 7II

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ATOM  1925  CD  GLU A 246      9.544  56.818  53.737  1.00 25.63      A   C
ATOM  1926  OE1 GLU A 246      8.335  56.577  53.927  1.00 24.93      A   O
ATOM  1927  OE2 GLU A 246     10.444  56.423  54.508  1.00 27.10      A   O
ATOM  1928  C   GLU A 246      9.324  56.714  48.828  1.00 15.72      A   C
ATOM  1929  O   GLU A 246      9.691  55.589  48.494  1.00 15.40      A   O
ATOM  1930  N   ARG A 247      8.326  57.359  48.235  1.00 16.57      A   N
ATOM  1931  CA  ARG A 247      7.611  56.790  47.105  1.00 18.74      A   C
ATOM  1932  CB  ARG A 247      6.445  57.710  46.711  1.00 23.10      A   C
ATOM  1933  CG  ARG A 247      5.875  57.451  45.325  1.00 32.32      A   C
ATOM  1934  CD  ARG A 247      4.561  58.204  45.114  1.00 40.32      A   C
ATOM  1935  NE  ARG A 247      4.084  58.117  43.733  1.00 47.44      A   N
ATOM  1936  CZ  ARG A 247      4.569  58.835  42.722  1.00 49.78      A   C
ATOM  1937  NH1 ARG A 247      5.548  59.705  42.931  1.00 51.70      A   N
ATOM  1938  NH2 ARG A 247      4.079  58.682  41.497  1.00 52.43      A   N
ATOM  1939  C   ARG A 247      8.594  56.630  45.941  1.00 17.54      A   C
ATOM  1940  O   ARG A 247      8.654  55.578  45.299  1.00 14.31      A   O
ATOM  1941  N   GLN A 248      9.375  57.672  45.677  1.00 15.93      A   N
ATOM  1942  CA  GLN A 248     10.350  57.608  44.598  1.00 16.24      A   C
ATOM  1943  CB  GLN A 248     11.120  58.929  44.485  1.00 17.33      A   C
ATOM  1944  CG  GLN A 248     10.267  60.119  44.047  1.00 16.22      A   C
ATOM  1945  CD  GLN A 248      9.552  59.879  42.725  1.00 22.44      A   C
ATOM  1946  OE1 GLN A 248     10.184  59.627  41.694  1.00 22.85      A   O
ATOM  1947  NE2 GLN A 248      8.225  59.958  42.749  1.00 24.90      A   N
ATOM  1948  C   GLN A 248     11.324  56.453  44.815  1.00 15.90      A   C
ATOM  1949  O   GLN A 248     11.705  55.768  43.866  1.00 16.87      A   O
ATOM  1950  N   ALA A 249     11.720  56.231  46.065  1.00 15.92      A   N
ATOM  1951  CA  ALA A 249     12.644  55.146  46.384  1.00 15.55      A   C
ATOM  1952  CB  ALA A 249     13.015  55.191  47.857  1.00 16.80      A   C
ATOM  1953  C   ALA A 249     12.032  53.789  46.041  1.00 16.47      A   C
ATOM  1954  O   ALA A 249     12.685  52.943  45.426  1.00 16.21      A   O
ATOM  1955  N   LYS A 250     10.779  53.582  46.438  1.00 16.38      A   N
ATOM  1956  CA  LYS A 250     10.102  52.316  46.159  1.00 18.81      A   C
ATOM  1957  CB  LYS A 250      8.750  52.258  46.880  1.00 20.86      A   C
ATOM  1958  CG  LYS A 250      8.843  52.132  48.394  1.00 26.84      A   C
ATOM  1959  CD  LYS A 250      7.488  51.745  48.988  1.00 31.08      A   C
ATOM  1960  CE  LYS A 250      7.554  51.607  50.507  1.00 31.43      A   C
ATOM  1961  NZ  LYS A 250      7.896  52.899  51.156  1.00 29.87      A   N
ATOM  1962  C   LYS A 250      9.884  52.121  44.661  1.00 18.41      A   C
ATOM  1963  O   LYS A 250     10.073  51.024  44.125  1.00 15.17      A   O
ATOM  1964  N   GLU A 251      9.493  53.200  43.992  1.00 15.62      A   N
ATOM  1965  CA  GLU A 251      9.224  53.167  42.562  1.00 18.32      A   C
ATOM  1966  CB  GLU A 251      8.586  54.486  42.119  1.00 20.33      A   C
ATOM  1967  CG  GLU A 251      7.205  54.758  42.692  1.00 23.48      A   C
ATOM  1968  CD  GLU A 251      6.106  54.036  41.936  1.00 25.23      A   C
ATOM  1969  OE1 GLU A 251      6.415  53.361  40.932  1.00 28.49      A   O
ATOM  1970  OE2 GLU A 251      4.932  54.152  42.341  1.00 25.47      A   O
ATOM  1971  C   GLU A 251     10.448  52.921  41.694  1.00 20.06      A   C
ATOM  1972  O   GLU A 251     10.398  52.121  40.763  1.00 17.23      A   O
ATOM  1973  N   TRP A 252     11.547  53.606  41.997  1.00 19.52      A   N
ATOM  1974  CA  TRP A 252     12.748  53.489  41.175  1.00 20.14      A   C
ATOM  1975  CB  TRP A 252     13.276  54.885  40.832  1.00 18.05      A   C
ATOM  1976  CG  TRP A 252     12.305  55.710  40.043  1.00 18.22      A   C
ATOM  1977  CD2 TRP A 252     12.039  55.607  38.640  1.00 20.57      A   C
ATOM  1978  CE2 TRP A 252     11.017  56.533  38.339  1.00 20.85      A   C
ATOM  1979  CE3 TRP A 252     12.564  54.818  37.607  1.00 21.87      A   C
ATOM  1980  CD1 TRP A 252     11.460  56.669  40.523  1.00 17.88      A   C
ATOM  1981  NE1 TRP A 252     10.683  57.168  39.508  1.00 17.77      A   N
ATOM  1982  CZ2 TRP A 252     10.506  56.697  37.041  1.00 22.03      A   C
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Figure 7JJ

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ATOM  1983 CZ3 TRP A 252     12.055  54.978  36.314  1.00 21.57    A   C
ATOM  1984 CH2 TRP A 252     11.036  55.913  36.045  1.00 22.86    A   C
ATOM  1985 C   TRP A 252     13.902  52.641  41.688  1.00 22.39    A   C
ATOM  1986 O   TRP A 252     14.680  52.122  40.886  1.00 23.72    A   O
ATOM  1987 N   LEU A 253     14.024  52.504  43.003  1.00 22.18    A   N
ATOM  1988 CA  LEU A 253     15.106  51.717  43.588  1.00 25.35    A   C
ATOM  1989 CB  LEU A 253     15.809  52.524  44.680  1.00 20.44    A   C
ATOM  1990 CG  LEU A 253     16.355  53.904  44.285  1.00 21.92    A   C
ATOM  1991 CD1 LEU A 253     16.785  54.649  45.532  1.00 18.63    A   C
ATOM  1992 CD2 LEU A 253     17.530  53.758  43.316  1.00 20.79    A   C
ATOM  1993 C   LEU A 253     14.583  50.401  44.168  1.00 29.73    A   C
ATOM  1994 O   LEU A 253     15.357  49.570  44.647  1.00 31.04    A   O
ATOM  1995 N   LYS A 254     13.267  50.219  44.121  1.00 33.91    A   N
ATOM  1996 CA  LYS A 254     12.638  49.007  44.631  1.00 39.79    A   C
ATOM  1997 CB  LYS A 254     13.102  47.795  43.812  1.00 43.18    A   C
ATOM  1998 CG  LYS A 254     12.330  46.518  44.102  1.00 51.27    A   C
ATOM  1999 CD  LYS A 254     12.747  45.377  43.181  1.00 56.67    A   C
ATOM  2000 CE  LYS A 254     11.928  44.121  43.464  1.00 59.29    A   C
ATOM  2001 NZ  LYS A 254     10.463  44.368  43.307  1.00 62.20    A   N
ATOM  2002 C   LYS A 254     12.967  48.805  46.110  1.00 41.24    A   C
ATOM  2003 O   LYS A 254     13.111  47.678  46.586  1.00 42.02    A   O
ATOM  2004 N   LEU A 255     13.091  49.911  46.834  1.00 42.21    A   N
ATOM  2005 CA  LEU A 255     13.396  49.856  48.255  1.00 43.88    A   C
ATOM  2006 CB  LEU A 255     14.643  50.687  48.560  1.00 41.85    A   C
ATOM  2007 CG  LEU A 255     15.934  50.186  47.910  1.00 40.40    A   C
ATOM  2008 CD1 LEU A 255     17.065  51.143  48.229  1.00 40.11    A   C
ATOM  2009 CD2 LEU A 255     16.258  48.788  48.412  1.00 39.40    A   C
ATOM  2010 C   LEU A 255     12.211  50.365  49.070  1.00 46.21    A   C
ATOM  2011 O   LEU A 255     12.350  51.427  49.715  1.00 47.30    A   O
ATOM  2012 OXT LEU A 255     11.152  49.696  49.044  1.00 48.09    A   O
ATOM  2013 CB  MET B   1      3.272 103.508  55.905  1.00 23.27    B   C
ATOM  2014 CG  MET B   1      3.026 102.116  56.484  1.00 25.31    B   C
ATOM  2015 SD  MET B   1      1.613 101.253  55.747  1.00 29.32    B   S
ATOM  2016 CE  MET B   1      0.239 102.076  56.594  1.00 27.48    B   C
ATOM  2017 C   MET B   1      5.739 103.357  56.203  1.00 22.82    B   C
ATOM  2018 O   MET B   1      6.391 103.503  55.166  1.00 21.44    B   O
ATOM  2019 N   MET B   1      4.661 105.565  55.875  1.00 22.28    B   N
ATOM  2020 CA  MET B   1      4.509 104.211  56.478  1.00 22.89    B   C
ATOM  2021 N   LYS B   2      6.057 102.479  57.148  1.00 22.63    B   N
ATOM  2022 CA  LYS B   2      7.185 101.568  57.010  1.00 21.27    B   C
ATOM  2023 CB  LYS B   2      8.060 101.591  58.260  1.00 21.29    B   C
ATOM  2024 CG  LYS B   2      9.273 100.675  58.156  1.00 18.62    B   C
ATOM  2025 CD  LYS B   2     10.097 100.705  59.419  1.00 18.80    B   C
ATOM  2026 CE  LYS B   2     11.414  99.983  59.213  1.00 19.94    B   C
ATOM  2027 NZ  LYS B   2     12.203  99.908  60.474  1.00 21.20    B   N
ATOM  2028 C   LYS B   2      6.610 100.169  56.822  1.00 19.67    B   C
ATOM  2029 O   LYS B   2      5.903  99.661  57.692  1.00 20.03    B   O
ATOM  2030 N   ILE B   3      6.915  99.545  55.689  1.00 18.60    B   N
ATOM  2031 CA  ILE B   3      6.395  98.213  55.410  1.00 16.13    B   C
ATOM  2032 CB  ILE B   3      5.409  98.250  54.232  1.00 18.20    B   C
ATOM  2033 CG2 ILE B   3      4.281  99.237  54.516  1.00 15.72    B   C
ATOM  2034 CG1 ILE B   3      6.156  98.669  52.964  1.00 17.99    B   C
ATOM  2035 CD1 ILE B   3      5.909  97.772  51.772  1.00 20.13    B   C
ATOM  2036 C   ILE B   3      7.476  97.190  55.062  1.00 17.01    B   C
ATOM  2037 O   ILE B   3      8.637  97.535  54.820  1.00 13.35    B   O
ATOM  2038 N   GLY B   4      7.072  95.924  55.046  1.00 15.79    B   N
ATOM  2039 CA  GLY B   4      7.982  94.859  54.678  1.00 13.12    B   C
ATOM  2040 C   GLY B   4      7.474  94.217  53.401  1.00 12.84    B   C
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Figure 7KK

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ATOM  2041  O   GLY B  4      6.271  94.248  53.123  1.00 12.27    B   O
ATOM  2042  N   VAL B  5      8.387  93.670  52.602  1.00 11.41    B   N
ATOM  2043  CA  VAL B  5      8.024  92.982  51.362  1.00 12.46    B   C
ATOM  2044  CB  VAL B  5      8.471  93.755  50.092  1.00 11.43    B   C
ATOM  2045  CG1 VAL B  5      8.281  92.886  48.860  1.00 10.57    B   C
ATOM  2046  CG2 VAL B  5      7.646  95.026  49.938  1.00 13.41    B   C
ATOM  2047  C   VAL B  5      8.745  91.641  51.404  1.00 11.84    B   C
ATOM  2048  O   VAL B  5      9.964  91.591  51.565  1.00 13.84    B   O
ATOM  2049  N   PHE B  6      7.989  90.559  51.277  1.00 11.52    B   N
ATOM  2050  CA  PHE B  6      8.571  89.222  51.330  1.00 12.00    B   C
ATOM  2051  CB  PHE B  6      7.930  88.429  52.471  1.00 14.01    B   C
ATOM  2052  CG  PHE B  6      8.313  86.975  52.485  1.00 15.68    B   C
ATOM  2053  CD1 PHE B  6      9.650  86.598  52.576  1.00 15.79    B   C
ATOM  2054  CD2 PHE B  6      7.340  85.983  52.403  1.00 17.28    B   C
ATOM  2055  CE1 PHE B  6     10.017  85.251  52.584  1.00 15.22    B   C
ATOM  2056  CE2 PHE B  6      7.699  84.628  52.411  1.00 18.59    B   C
ATOM  2057  CZ  PHE B  6      9.044  84.268  52.502  1.00 15.23    B   C
ATOM  2058  C   PHE B  6      8.440  88.410  50.046  1.00 12.99    B   C
ATOM  2059  O   PHE B  6      7.396  88.412  49.400  1.00 13.52    B   O
ATOM  2060  N   ASP B  7      9.512  87.707  49.695  1.00 13.22    B   N
ATOM  2061  CA  ASP B  7      9.533  86.839  48.523  1.00 12.28    B   C
ATOM  2062  CB  ASP B  7      9.914  87.600  47.254  1.00 12.10    B   C
ATOM  2063  CG  ASP B  7      9.838  86.727  46.018  1.00 11.16    B   C
ATOM  2064  OD1 ASP B  7      8.773  86.111  45.800  1.00 11.05    B   O
ATOM  2065  OD2 ASP B  7     10.835  86.652  45.265  1.00 15.46    B   O
ATOM  2066  C   ASP B  7     10.544  85.730  48.749  1.00 12.97    B   C
ATOM  2067  O   ASP B  7     11.402  85.831  49.626  1.00 14.91    B   O
ATOM  2068  N   SER B  8     10.444  84.670  47.953  1.00 13.64    B   N
ATOM  2069  CA  SER B  8     11.367  83.551  48.076  1.00 13.32    B   C
ATOM  2070  CB  SER B  8     10.870  82.357  47.246  1.00 11.76    B   C
ATOM  2071  OG  SER B  8     10.643  82.716  45.892  1.00 12.59    B   O
ATOM  2072  C   SER B  8     12.760  83.979  47.618  1.00 12.86    B   C
ATOM  2073  O   SER B  8     13.760  83.328  47.931  1.00 15.56    B   O
ATOM  2074  N   GLY B  9     12.826  85.088  46.888  1.00 14.15    B   N
ATOM  2075  CA  GLY B  9     14.113  85.565  46.418  1.00 11.94    B   C
ATOM  2076  C   GLY B  9     14.060  86.923  45.751  1.00 13.28    B   C
ATOM  2077  O   GLY B  9     13.420  87.855  46.255  1.00 11.42    B   O
ATOM  2078  N   VAL B 10     14.731  87.031  44.608  1.00 11.70    B   N
ATOM  2079  CA  VAL B 10     14.793  88.283  43.848  1.00 13.19    B   C
ATOM  2080  CB  VAL B 10     16.035  88.301  42.931  1.00 11.94    B   C
ATOM  2081  CG1 VAL B 10     15.956  87.149  41.948  1.00 17.01    B   C
ATOM  2082  CG2 VAL B 10     16.148  89.633  42.200  1.00 12.63    B   C
ATOM  2083  C   VAL B 10     13.546  88.495  42.995  1.00 12.34    B   C
ATOM  2084  O   VAL B 10     13.267  89.604  42.550  1.00 14.01    B   O
ATOM  2085  N   GLY B 11     12.794  87.426  42.768  1.00 12.08    B   N
ATOM  2086  CA  GLY B 11     11.591  87.540  41.957  1.00 14.90    B   C
ATOM  2087  C   GLY B 11     10.634  88.640  42.373  1.00 12.77    B   C
ATOM  2088  O   GLY B 11     10.004  89.278  41.524  1.00 13.23    B   O
ATOM  2089  N   GLY B 12     10.524  88.861  43.679  1.00 13.56    B   N
ATOM  2090  CA  GLY B 12      9.639  89.887  44.198  1.00 15.76    B   C
ATOM  2091  C   GLY B 12      9.917  91.279  43.659  1.00 15.26    B   C
ATOM  2092  O   GLY B 12      9.141  92.213  43.899  1.00 15.12    B   O
ATOM  2093  N   PHE B 13     11.024  91.426  42.937  1.00 12.59    B   N
ATOM  2094  CA  PHE B 13     11.376  92.713  42.360  1.00 14.03    B   C
ATOM  2095  CB  PHE B 13     12.702  92.620  41.589  1.00 14.04    B   C
ATOM  2096  CG  PHE B 13     13.929  92.823  42.446  1.00 14.87    B   C
ATOM  2097  CD1 PHE B 13     15.133  93.231  41.868  1.00 16.32    B   C
ATOM  2098  CD2 PHE B 13     13.883  92.629  43.823  1.00 14.64    B   C
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Figure 7LL

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ATOM  2099 CE1 PHE B 13     16.272  93.448  42.651  1.00 13.70    B   C
ATOM  2100 CE2 PHE B 13     15.013  92.842  44.614  1.00 13.54    B   C
ATOM  2101 CZ  PHE B 13     16.210  93.254  44.025  1.00 15.35    B   C
ATOM  2102 C   PHE B 13     10.260  93.184  41.425  1.00 14.72    B   C
ATOM  2103 O   PHE B 13     10.013  94.380  41.301  1.00 12.42    B   O
ATOM  2104 N   SER B 14      9.580  92.243  40.775  1.00 14.71    B   N
ATOM  2105 CA  SER B 14      8.494  92.600  39.860  1.00 14.65    B   C
ATOM  2106 CB  SER B 14      7.918  91.349  39.187  1.00 14.09    B   C
ATOM  2107 OG  SER B 14      7.405  90.436  40.135  1.00 13.06    B   O
ATOM  2108 C   SER B 14      7.380  93.355  40.587  1.00 14.07    B   C
ATOM  2109 O   SER B 14      6.688  94.187  39.994  1.00 13.89    B   O
ATOM  2110 N   VAL B 15      7.212  93.064  41.872  1.00 14.55    B   N
ATOM  2111 CA  VAL B 15      6.196  93.737  42.675  1.00 14.09    B   C
ATOM  2112 CB  VAL B 15      5.675  92.827  43.814  1.00 12.74    B   C
ATOM  2113 CG1 VAL B 15      4.705  93.600  44.698  1.00 13.09    B   C
ATOM  2114 CG2 VAL B 15      4.971  91.604  43.224  1.00 11.77    B   C
ATOM  2115 C   VAL B 15      6.789  95.003  43.283  1.00 14.70    B   C
ATOM  2116 O   VAL B 15      6.145  96.052  43.307  1.00 13.74    B   O
ATOM  2117 N   LEU B 16      8.022  94.903  43.769  1.00 13.69    B   N
ATOM  2118 CA  LEU B 16      8.679  96.048  44.384  1.00 14.26    B   C
ATOM  2119 CB  LEU B 16     10.082  95.662  44.863  1.00 13.66    B   C
ATOM  2120 CG  LEU B 16     10.940  96.793  45.448  1.00 14.21    B   C
ATOM  2121 CD1 LEU B 16     10.201  97.451  46.605  1.00 12.59    B   C
ATOM  2122 CD2 LEU B 16     12.280  96.242  45.905  1.00 12.19    B   C
ATOM  2123 C   LEU B 16      8.757  97.212  43.401  1.00 16.29    B   C
ATOM  2124 O   LEU B 16      8.614  98.373  43.787  1.00 16.57    B   O
ATOM  2125 N   LYS B 17      8.984  96.896  42.129  1.00 17.51    B   N
ATOM  2126 CA  LYS B 17      9.069  97.927  41.099  1.00 19.45    B   C
ATOM  2127 CB  LYS B 17      9.349  97.298  39.733  1.00 19.95    B   C
ATOM  2128 CG  LYS B 17      9.302  98.291  38.578  1.00 24.40    B   C
ATOM  2129 CD  LYS B 17      9.568  97.608  37.245  1.00 29.79    B   C
ATOM  2130 CE  LYS B 17      9.472  98.586  36.081  1.00 33.15    B   C
ATOM  2131 NZ  LYS B 17      9.808  97.925  34.784  1.00 35.04    B   N
ATOM  2132 C   LYS B 17      7.769  98.722  41.038  1.00 19.40    B   C
ATOM  2133 O   LYS B 17      7.788  99.950  40.985  1.00 18.81    B   O
ATOM  2134 N   SER B 18      6.642  98.018  41.042  1.00 18.29    B   N
ATOM  2135 CA  SER B 18      5.344  98.675  40.997  1.00 18.21    B   C
ATOM  2136 CB  SER B 18      4.221  97.636  40.941  1.00 17.21    B   C
ATOM  2137 OG  SER B 18      4.357  96.808  39.798  1.00 17.80    B   O
ATOM  2138 C   SER B 18      5.162  99.561  42.222  1.00 19.88    B   C
ATOM  2139 O   SER B 18      4.720 100.703  42.112  1.00 17.77    B   O
ATOM  2140 N   LEU B 19      5.510  99.030  43.391  1.00 19.41    B   N
ATOM  2141 CA  LEU B 19      5.379  99.785  44.629  1.00 19.33    B   C
ATOM  2142 CB  LEU B 19      5.839  98.936  45.817  1.00 18.90    B   C
ATOM  2143 CG  LEU B 19      5.085  97.622  46.027  1.00 20.11    B   C
ATOM  2144 CD1 LEU B 19      5.701  96.850  47.188  1.00 18.40    B   C
ATOM  2145 CD2 LEU B 19      3.612  97.919  46.289  1.00 17.29    B   C
ATOM  2146 C   LEU B 19      6.205 101.063  44.564  1.00 18.96    B   C
ATOM  2147 O   LEU B 19      5.722 102.145  44.897  1.00 19.77    B   O
ATOM  2148 N   LEU B 20      7.455 100.930  44.136  1.00 19.62    B   N
ATOM  2149 CA  LEU B 20      8.355 102.071  44.024  1.00 20.54    B   C
ATOM  2150 CB  LEU B 20      9.736 101.605  43.548  1.00 19.03    B   C
ATOM  2151 CG  LEU B 20     10.562 100.763  44.529  1.00 21.61    B   C
ATOM  2152 CD1 LEU B 20     11.789 100.217  43.824  1.00 17.66    B   C
ATOM  2153 CD2 LEU B 20     10.968 101.613  45.731  1.00 17.70    B   C
ATOM  2154 C   LEU B 20      7.821 103.148  43.077  1.00 21.80    B   C
ATOM  2155 O   LEU B 20      7.864 104.334  43.397  1.00 24.32    B   O
ATOM  2156 N   LYS B 21      7.321 102.736  41.916  1.00 22.92    B   N
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Figure 7MM

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ATOM  2157 CA  LYS B 21      6.789 103.680  40.932  1.00 25.60    B   C
ATOM  2158 CB  LYS B 21      6.334 102.934  39.671  1.00 29.64    B   C
ATOM  2159 CG  LYS B 21      7.412 102.050  39.049  1.00 39.78    B   C
ATOM  2160 CD  LYS B 21      6.819 100.964  38.139  1.00 45.78    B   C
ATOM  2161 CE  LYS B 21      6.314 101.521  36.813  1.00 49.52    B   C
ATOM  2162 NZ  LYS B 21      7.428 101.970  35.926  1.00 52.40    B   N
ATOM  2163 C   LYS B 21      5.610 104.455  41.513  1.00 24.12    B   C
ATOM  2164 O   LYS B 21      5.461 105.652  41.270  1.00 21.99    B   O
ATOM  2165 N   ALA B 22      4.775 103.762  42.281  1.00 22.32    B   N
ATOM  2166 CA  ALA B 22      3.602 104.378  42.889  1.00 23.02    B   C
ATOM  2167 CB  ALA B 22      2.619 103.299  43.321  1.00 21.51    B   C
ATOM  2168 C   ALA B 22      3.950 105.279  44.074  1.00 25.48    B   C
ATOM  2169 O   ALA B 22      3.082 105.975  44.602  1.00 26.34    B   O
ATOM  2170 N   ARG B 23      5.214 105.264  44.489  1.00 26.06    B   N
ATOM  2171 CA  ARG B 23      5.674 106.090  45.606  1.00 28.97    B   C
ATOM  2172 CB  ARG B 23      5.794 107.556  45.170  1.00 33.33    B   C
ATOM  2173 CG  ARG B 23      6.504 107.770  43.850  1.00 41.37    B   C
ATOM  2174 CD  ARG B 23      6.349 109.205  43.378  1.00 47.44    B   C
ATOM  2175 NE  ARG B 23      6.782 109.366  41.992  1.00 56.48    B   N
ATOM  2176 CZ  ARG B 23      6.602 110.472  41.275  1.00 59.85    B   C
ATOM  2177 NH1 ARG B 23      5.998 111.520  41.819  1.00 63.01    B   N
ATOM  2178 NH2 ARG B 23      7.019 110.529  40.015  1.00 61.13    B   N
ATOM  2179 C   ARG B 23      4.697 106.012  46.774  1.00 27.89    B   C
ATOM  2180 O   ARG B 23      4.246 107.042  47.276  1.00 27.91    B   O
ATOM  2181 N   LEU B 24      4.373 104.797  47.205  1.00 25.94    B   N
ATOM  2182 CA  LEU B 24      3.430 104.611  48.303  1.00 24.48    B   C
ATOM  2183 CB  LEU B 24      2.653 103.301  48.118  1.00 22.57    B   C
ATOM  2184 CG  LEU B 24      1.822 103.103  46.847  1.00 24.84    B   C
ATOM  2185 CD1 LEU B 24      1.067 101.779  46.942  1.00 23.08    B   C
ATOM  2186 CD2 LEU B 24      0.842 104.266  46.671  1.00 23.49    B   C
ATOM  2187 C   LEU B 24      4.048 104.617  49.699  1.00 24.22    B   C
ATOM  2188 O   LEU B 24      3.445 105.126  50.641  1.00 25.35    B   O
ATOM  2189 N   PHE B 25      5.250 104.068  49.842  1.00 25.14    B   N
ATOM  2190 CA  PHE B 25      5.865 103.997  51.161  1.00 25.20    B   C
ATOM  2191 CB  PHE B 25      6.078 102.531  51.530  1.00 24.64    B   C
ATOM  2192 CG  PHE B 25      4.886 101.665  51.251  1.00 23.70    B   C
ATOM  2193 CD1 PHE B 25      4.849 100.851  50.123  1.00 23.04    B   C
ATOM  2194 CD2 PHE B 25      3.788 101.685  52.098  1.00 22.47    B   C
ATOM  2195 CE1 PHE B 25      3.729 100.070  49.845  1.00 20.01    B   C
ATOM  2196 CE2 PHE B 25      2.666 100.910  51.828  1.00 22.66    B   C
ATOM  2197 CZ  PHE B 25      2.637 100.100  50.697  1.00 21.24    B   C
ATOM  2198 C   PHE B 25      7.164 104.758  51.361  1.00 25.96    B   C
ATOM  2199 O   PHE B 25      8.020 104.796  50.482  1.00 28.54    B   O
ATOM  2200 N   ASP B 26      7.308 105.355  52.540  1.00 26.35    B   N
ATOM  2201 CA  ASP B 26      8.512 106.108  52.872  1.00 28.67    B   C
ATOM  2202 CB  ASP B 26      8.300 106.958  54.130  1.00 31.57    B   C
ATOM  2203 CG  ASP B 26      7.335 108.101  53.907  1.00 33.21    B   C
ATOM  2204 OD1 ASP B 26      7.429 108.753  52.844  1.00 33.40    B   O
ATOM  2205 OD2 ASP B 26      6.495 108.352  54.800  1.00 37.72    B   O
ATOM  2206 C   ASP B 26      9.697 105.186  53.109  1.00 25.51    B   C
ATOM  2207 O   ASP B 26     10.840 105.567  52.877  1.00 22.85    B   O
ATOM  2208 N   GLU B 27      9.421 103.974  53.581  1.00 24.08    B   N
ATOM  2209 CA  GLU B 27     10.483 103.013  53.859  1.00 21.60    B   C
ATOM  2210 CB  GLU B 27     10.964 103.179  55.305  1.00 22.98    B   C
ATOM  2211 CG  GLU B 27     11.869 102.071  55.800  1.00 25.73    B   C
ATOM  2212 CD  GLU B 27     12.636 102.459  57.051  1.00 30.40    B   C
ATOM  2213 OE1 GLU B 27     12.088 103.219  57.883  1.00 28.18    B   O
ATOM  2214 OE2 GLU B 27     13.785 101.993  57.207  1.00 28.75    B   O
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Figure 7NN

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ATOM  2215 C   GLU B 27    10.036 101.576  53.601  1.00 19.70    B   C
ATOM  2216 O   GLU B 27     8.919 101.184  53.948  1.00 17.68    B   O
ATOM  2217 N   ILE B 28    10.926 100.795  52.995  1.00 16.91    B   N
ATOM  2218 CA  ILE B 28    10.630  99.407  52.651  1.00 14.07    B   C
ATOM  2219 CB  ILE B 28    10.394  99.276  51.121  1.00 15.11    B   C
ATOM  2220 CG2 ILE B 28    10.279  97.816  50.711  1.00 15.06    B   C
ATOM  2221 CG1 ILE B 28     9.124 100.034  50.732  1.00 15.08    B   C
ATOM  2222 CD1 ILE B 28     8.920 100.162  49.218  1.00 17.55    B   C
ATOM  2223 C   ILE B 28    11.740  98.446  53.069  1.00 14.73    B   C
ATOM  2224 O   ILE B 28    12.925  98.694  52.825  1.00 14.43    B   O
ATOM  2225 N   ILE B 29    11.348  97.357  53.720  1.00 13.73    B   N
ATOM  2226 CA  ILE B 29    12.299  96.338  54.143  1.00 15.11    B   C
ATOM  2227 CB  ILE B 29    12.113  95.957  55.636  1.00 14.64    B   C
ATOM  2228 CG2 ILE B 29    13.231  95.012  56.077  1.00 13.07    B   C
ATOM  2229 CG1 ILE B 29    12.129  97.214  56.521  1.00 16.50    B   C
ATOM  2230 CD1 ILE B 29    13.462  97.949  56.554  1.00 12.57    B   C
ATOM  2231 C   ILE B 29    11.989  95.121  53.262  1.00 14.26    B   C
ATOM  2232 O   ILE B 29    10.960  94.460  53.438  1.00 16.06    B   O
ATOM  2233 N   TYR B 30    12.857  94.855  52.293  1.00 12.97    B   N
ATOM  2234 CA  TYR B 30    12.667  93.728  51.382  1.00 12.66    B   C
ATOM  2235 CB  TYR B 30    13.095  94.117  49.957  1.00 11.95    B   C
ATOM  2236 CG  TYR B 30    12.831  93.042  48.913  1.00 11.71    B   C
ATOM  2237 CD1 TYR B 30    11.703  93.097  48.096  1.00  9.69    B   C
ATOM  2238 CE1 TYR B 30    11.441  92.100  47.149  1.00 12.54    B   C
ATOM  2239 CD2 TYR B 30    13.700  91.958  48.762  1.00 12.15    B   C
ATOM  2240 CE2 TYR B 30    13.449  90.953  47.817  1.00 14.27    B   C
ATOM  2241 CZ  TYR B 30    12.319  91.033  47.014  1.00 14.57    B   C
ATOM  2242 OH  TYR B 30    12.078  90.061  46.070  1.00 11.66    B   O
ATOM  2243 C   TYR B 30    13.473  92.516  51.842  1.00 15.13    B   C
ATOM  2244 O   TYR B 30    14.673  92.624  52.115  1.00 17.82    B   O
ATOM  2245 N   TYR B 31    12.812  91.364  51.932  1.00 13.53    B   N
ATOM  2246 CA  TYR B 31    13.488  90.144  52.350  1.00 13.30    B   C
ATOM  2247 CB  TYR B 31    13.063  89.742  53.773  1.00 14.35    B   C
ATOM  2248 CG  TYR B 31    13.588  88.381  54.209  1.00 13.93    B   C
ATOM  2249 CD1 TYR B 31    14.955  88.143  54.318  1.00 13.81    B   C
ATOM  2250 CE1 TYR B 31    15.446  86.887  54.682  1.00 16.52    B   C
ATOM  2251 CD2 TYR B 31    12.712  87.326  54.481  1.00 15.49    B   C
ATOM  2252 CE2 TYR B 31    13.191  86.064  54.850  1.00 17.62    B   C
ATOM  2253 CZ  TYR B 31    14.563  85.852  54.946  1.00 14.49    B   C
ATOM  2254 OH  TYR B 31    15.047  84.611  55.304  1.00 14.75    B   O
ATOM  2255 C   TYR B 31    13.188  89.005  51.382  1.00 11.69    B   C
ATOM  2256 O   TYR B 31    12.032  88.657  51.153  1.00 12.79    B   O
ATOM  2257 N   GLY B 32    14.246  88.440  50.812  1.00 12.78    B   N
ATOM  2258 CA  GLY B 32    14.093  87.327  49.896  1.00 11.28    B   C
ATOM  2259 C   GLY B 32    14.761  86.117  50.522  1.00 13.78    B   C
ATOM  2260 O   GLY B 32    15.950  86.162  50.839  1.00 11.17    B   O
ATOM  2261 N   ASP B 33    14.002  85.040  50.710  1.00 14.25    B   N
ATOM  2262 CA  ASP B 33    14.540  83.819  51.306  1.00 15.29    B   C
ATOM  2263 CB  ASP B 33    13.391  82.987  51.885  1.00 13.57    B   C
ATOM  2264 CG  ASP B 33    13.871  81.730  52.589  1.00 14.42    B   C
ATOM  2265 OD1 ASP B 33    15.034  81.702  53.046  1.00 14.38    B   O
ATOM  2266 OD2 ASP B 33    13.077  80.773  52.695  1.00 14.44    B   O
ATOM  2267 C   ASP B 33    15.288  83.049  50.226  1.00 14.09    B   C
ATOM  2268 O   ASP B 33    15.027  81.867  49.980  1.00 12.43    B   O
ATOM  2269 N   SER B 34    16.238  83.739  49.597  1.00 14.94    B   N
ATOM  2270 CA  SER B 34    17.016  83.186  48.490  1.00 14.92    B   C
ATOM  2271 CB  SER B 34    17.941  84.268  47.908  1.00 13.20    B   C
ATOM  2272 OG  SER B 34    18.886  84.714  48.863  1.00 14.39    B   O
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Figure 7OO

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ATOM  2273  C   SER B  34     17.821  81.924  48.772  1.00 14.53      B   C
ATOM  2274  O   SER B  34     18.348  81.308  47.849  1.00 12.91      B   O
ATOM  2275  N   ALA B  35     17.930  81.535  50.034  1.00 13.97      B   N
ATOM  2276  CA  ALA B  35     18.664  80.317  50.345  1.00 15.25      B   C
ATOM  2277  CB  ALA B  35     19.050  80.297  51.820  1.00 15.69      B   C
ATOM  2278  C   ALA B  35     17.801  79.101  50.023  1.00 15.43      B   C
ATOM  2279  O   ALA B  35     18.321  78.010  49.776  1.00 13.55      B   O
ATOM  2280  N   ARG B  36     16.484  79.296  50.000  1.00 13.78      B   N
ATOM  2281  CA  ARG B  36     15.567  78.185  49.777  1.00 14.22      B   C
ATOM  2282  CB  ARG B  36     14.697  78.023  51.027  1.00 13.17      B   C
ATOM  2283  CG  ARG B  36     15.541  77.986  52.303  1.00 13.84      B   C
ATOM  2284  CD  ARG B  36     14.775  77.513  53.520  1.00 16.20      B   C
ATOM  2285  NE  ARG B  36     13.830  78.511  54.012  1.00 13.15      B   N
ATOM  2286  CZ  ARG B  36     13.310  78.500  55.235  1.00 14.54      B   C
ATOM  2287  NH1 ARG B  36     13.642  77.542  56.090  1.00 13.26      B   N
ATOM  2288  NH2 ARG B  36     12.468  79.454  55.613  1.00 15.47      B   N
ATOM  2289  C   ARG B  36     14.703  78.235  48.517  1.00 14.96      B   C
ATOM  2290  O   ARG B  36     13.971  77.288  48.220  1.00 16.93      B   O
ATOM  2291  N   VAL B  37     14.791  79.328  47.770  1.00 14.56      B   N
ATOM  2292  CA  VAL B  37     14.036  79.461  46.530  1.00 15.83      B   C
ATOM  2293  CB  VAL B  37     14.327  80.840  45.875  1.00 16.33      B   C
ATOM  2294  CG1 VAL B  37     15.775  80.909  45.422  1.00 16.98      B   C
ATOM  2295  CG2 VAL B  37     13.379  81.093  44.719  1.00 16.47      B   C
ATOM  2296  C   VAL B  37     14.452  78.312  45.587  1.00 14.68      B   C
ATOM  2297  O   VAL B  37     15.615  77.895  45.575  1.00 15.45      B   O
ATOM  2298  N   PRO B  38     13.511  77.780  44.790  1.00 14.64      B   N
ATOM  2299  CD  PRO B  38     13.845  76.783  43.755  1.00 11.60      B   C
ATOM  2300  CA  PRO B  38     12.102  78.160  44.696  1.00 14.93      B   C
ATOM  2301  CB  PRO B  38     11.743  77.754  43.271  1.00 13.51      B   C
ATOM  2302  CG  PRO B  38     12.485  76.470  43.123  1.00 15.17      B   C
ATOM  2303  C   PRO B  38     11.191  77.489  45.710  1.00 15.27      B   C
ATOM  2304  O   PRO B  38     11.510  76.437  46.274  1.00 13.54      B   O
ATOM  2305  N   TYR B  39     10.043  78.118  45.915  1.00 13.69      B   N
ATOM  2306  CA  TYR B  39      9.013  77.623  46.811  1.00 13.90      B   C
ATOM  2307  CB  TYR B  39      8.268  78.798  47.444  1.00 13.72      B   C
ATOM  2308  CG  TYR B  39      8.922  79.471  48.624  1.00 10.70      B   C
ATOM  2309  CD1 TYR B  39     10.268  79.261  48.937  1.00 10.84      B   C
ATOM  2310  CE1 TYR B  39     10.860  79.906  50.023  1.00 12.25      B   C
ATOM  2311  CD2 TYR B  39      8.186  80.344  49.426  1.00 12.79      B   C
ATOM  2312  CE2 TYR B  39      8.766  80.996  50.514  1.00 12.39      B   C
ATOM  2313  CZ  TYR B  39     10.104  80.772  50.809  1.00 13.35      B   C
ATOM  2314  OH  TYR B  39     10.674  81.405  51.893  1.00 12.01      B   O
ATOM  2315  C   TYR B  39      7.997  76.821  45.987  1.00 14.02      B   C
ATOM  2316  O   TYR B  39      7.451  75.827  46.455  1.00 15.23      B   O
ATOM  2317  N   GLY B  40      7.752  77.290  44.765  1.00 16.75      B   N
ATOM  2318  CA  GLY B  40      6.768  76.686  43.874  1.00 16.84      B   C
ATOM  2319  C   GLY B  40      6.860  75.212  43.525  1.00 16.65      B   C
ATOM  2320  O   GLY B  40      5.886  74.620  43.049  1.00 14.08      B   O
ATOM  2321  N   THR B  41      8.017  74.611  43.766  1.00 15.91      B   N
ATOM  2322  CA  THR B  41      8.225  73.204  43.440  1.00 16.59      B   C
ATOM  2323  CB  THR B  41      9.636  72.990  42.900  1.00 16.07      B   C
ATOM  2324  OG1 THR B  41     10.580  73.477  43.861  1.00 15.88      B   O
ATOM  2325  CG2 THR B  41      9.817  73.737  41.592  1.00 19.86      B   C
ATOM  2326  C   THR B  41      8.072  72.320  44.659  1.00 16.87      B   C
ATOM  2327  O   THR B  41      8.245  71.099  44.584  1.00 18.68      B   O
ATOM  2328  N   LYS B  42      7.742  72.939  45.783  1.00 16.57      B   N
ATOM  2329  CA  LYS B  42      7.647  72.178  47.002  1.00 16.66      B   C
ATOM  2330  CB  LYS B  42      8.592  72.768  48.035  1.00 15.39      B   C
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Figure 7PP

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ATOM  2331  CG  LYS B  42      10.049  72.613  47.578  1.00 16.40      B   C
ATOM  2332  CD  LYS B  42      10.942  73.766  47.995  1.00 12.99      B   C
ATOM  2333  CE  LYS B  42      12.343  73.611  47.372  1.00 12.98      B   C
ATOM  2334  NZ  LYS B  42      13.246  74.754  47.688  1.00 12.01      B   N
ATOM  2335  C   LYS B  42       6.273  71.981  47.593  1.00 19.30      B   C
ATOM  2336  O   LYS B  42       5.311  72.659  47.234  1.00 19.46      B   O
ATOM  2337  N   ASP B  43       6.206  71.042  48.526  1.00 19.11      B   N
ATOM  2338  CA  ASP B  43       4.903  70.766  49.089  1.00 20.39      B   C
ATOM  2339  CB  ASP B  43       4.970  69.389  49.727  1.00 26.23      B   C
ATOM  2340  CG  ASP B  43       3.668  68.908  50.218  1.00 34.18      B   C
ATOM  2341  OD1 ASP B  43       3.032  69.628  51.023  1.00 35.73      B   O
ATOM  2342  OD2 ASP B  43       3.286  67.802  49.834  1.00 34.67      B   O
ATOM  2343  C   ASP B  43       4.324  71.860  50.037  1.00 18.74      B   C
ATOM  2344  O   ASP B  43       5.067  72.590  50.662  1.00 17.52      B   O
ATOM  2345  N   PRO B  44       2.970  71.973  50.139  1.00 16.86      B   N
ATOM  2346  CD  PRO B  44       1.945  71.249  49.366  1.00 16.70      B   C
ATOM  2347  CA  PRO B  44       2.316  72.976  51.001  1.00 15.67      B   C
ATOM  2348  CB  PRO B  44       0.838  72.608  50.910  1.00 16.57      B   C
ATOM  2349  CG  PRO B  44       0.714  72.164  49.520  1.00 15.09      B   C
ATOM  2350  C   PRO B  44       2.785  73.063  52.460  1.00 14.32      B   C
ATOM  2351  O   PRO B  44       2.975  74.159  52.984  1.00 14.18      B   O
ATOM  2352  N   THR B  45       2.968  71.928  53.125  1.00 12.56      B   N
ATOM  2353  CA  THR B  45       3.404  71.976  54.513  1.00 15.07      B   C
ATOM  2354  CB  THR B  45       3.416  70.544  55.159  1.00 14.56      B   C
ATOM  2355  OG1 THR B  45       3.473  70.671  56.582  1.00 20.74      B   O
ATOM  2356  CG2 THR B  45       4.617  69.725  54.690  1.00 16.79      B   C
ATOM  2357  C   THR B  45       4.773  72.673  54.661  1.00 13.75      B   C
ATOM  2358  O   THR B  45       5.015  73.370  55.644  1.00 15.18      B   O
ATOM  2359  N   THR B  46       5.652  72.512  53.675  1.00 14.31      B   N
ATOM  2360  CA  THR B  46       6.978  73.138  53.708  1.00 13.76      B   C
ATOM  2361  CB  THR B  46       7.908  72.534  52.625  1.00 15.70      B   C
ATOM  2362  OG1 THR B  46       8.111  71.139  52.888  1.00 16.08      B   O
ATOM  2363  CG2 THR B  46       9.257  73.237  52.611  1.00 14.55      B   C
ATOM  2364  C   THR B  46       6.874  74.645  53.463  1.00 14.40      B   C
ATOM  2365  O   THR B  46       7.538  75.450  54.120  1.00 12.91      B   O
ATOM  2366  N   ILE B  47       6.029  75.016  52.509  1.00 12.98      B   N
ATOM  2367  CA  ILE B  47       5.843  76.414  52.159  1.00 14.06      B   C
ATOM  2368  CB  ILE B  47       4.987  76.537  50.881  1.00 12.60      B   C
ATOM  2369  CG2 ILE B  47       4.790  78.005  50.517  1.00 13.35      B   C
ATOM  2370  CG1 ILE B  47       5.684  75.804  49.727  1.00 14.48      B   C
ATOM  2371  CD1 ILE B  47       4.831  75.660  48.469  1.00 13.95      B   C
ATOM  2372  C   ILE B  47       5.193  77.190  53.305  1.00 13.29      B   C
ATOM  2373  O   ILE B  47       5.588  78.314  53.610  1.00 12.68      B   O
ATOM  2374  N   LYS B  48       4.199  76.594  53.948  1.00 13.12      B   N
ATOM  2375  CA  LYS B  48       3.541  77.279  55.047  1.00 14.82      B   C
ATOM  2376  CB  LYS B  48       2.387  76.440  55.606  1.00 15.61      B   C
ATOM  2377  CG  LYS B  48       1.239  76.283  54.621  1.00 16.82      B   C
ATOM  2378  CD  LYS B  48       0.021  75.649  55.261  1.00 17.71      B   C
ATOM  2379  CE  LYS B  48      -1.123  75.558  54.259  1.00 21.58      B   C
ATOM  2380  NZ  LYS B  48      -2.370  75.047  54.891  1.00 23.95      B   N
ATOM  2381  C   LYS B  48       4.537  77.600  56.145  1.00 15.64      B   C
ATOM  2382  O   LYS B  48       4.546  78.719  56.661  1.00 14.41      B   O
ATOM  2383  N   GLN B  49       5.383  76.630  56.493  1.00 13.94      B   N
ATOM  2384  CA  GLN B  49       6.388  76.836  57.533  1.00 14.63      B   C
ATOM  2385  CB  GLN B  49       7.127  75.520  57.822  1.00 15.57      B   C
ATOM  2386  CG  GLN B  49       8.185  75.577  58.930  1.00 19.33      B   C
ATOM  2387  CD  GLN B  49       7.656  76.099  60.258  1.00 18.82      B   C
ATOM  2388  OE1 GLN B  49       6.509  75.840  60.638  1.00 17.48      B   O
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Figure 7QQ

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ATOM  2389 NE2 GLN B 49     8.498  76.826  60.977  1.00 19.58    B   N
ATOM  2390 C   GLN B 49     7.357  77.934  57.091  1.00 15.00    B   C
ATOM  2391 O   GLN B 49     7.754  78.773  57.898  1.00 15.49    B   O
ATOM  2392 N   PHE B 50     7.732  77.936  55.812  1.00 13.73    B   N
ATOM  2393 CA  PHE B 50     8.617  78.978  55.297  1.00 12.73    B   C
ATOM  2394 CB  PHE B 50     8.813  78.845  53.784  1.00 12.69    B   C
ATOM  2395 CG  PHE B 50     9.756  77.740  53.372  1.00 14.11    B   C
ATOM  2396 CD1 PHE B 50    10.540  77.073  54.310  1.00 13.47    B   C
ATOM  2397 CD2 PHE B 50     9.884  77.396  52.028  1.00 16.97    B   C
ATOM  2398 CE1 PHE B 50    11.442  76.080  53.915  1.00 14.96    B   C
ATOM  2399 CE2 PHE B 50    10.784  76.405  51.622  1.00 16.26    B   C
ATOM  2400 CZ  PHE B 50    11.563  75.747  52.569  1.00 13.12    B   C
ATOM  2401 C   PHE B 50     7.999  80.348  55.586  1.00 12.88    B   C
ATOM  2402 O   PHE B 50     8.690  81.281  55.998  1.00 14.04    B   O
ATOM  2403 N   GLY B 51     6.692  80.460  55.353  1.00 13.99    B   N
ATOM  2404 CA  GLY B 51     5.992  81.712  55.590  1.00 13.72    B   C
ATOM  2405 C   GLY B 51     6.023  82.158  57.043  1.00 14.83    B   C
ATOM  2406 O   GLY B 51     6.243  83.334  57.331  1.00 11.98    B   O
ATOM  2407 N   LEU B 52     5.788  81.227  57.966  1.00 15.32    B   N
ATOM  2408 CA  LEU B 52     5.815  81.555  59.388  1.00 18.38    B   C
ATOM  2409 CB  LEU B 52     5.525  80.320  60.248  1.00 18.53    B   C
ATOM  2410 CG  LEU B 52     4.074  79.939  60.511  1.00 24.25    B   C
ATOM  2411 CD1 LEU B 52     3.349  79.724  59.198  1.00 27.80    B   C
ATOM  2412 CD2 LEU B 52     4.037  78.679  61.371  1.00 26.46    B   C
ATOM  2413 C   LEU B 52     7.184  82.091  59.757  1.00 18.61    B   C
ATOM  2414 O   LEU B 52     7.303  83.096  60.455  1.00 21.72    B   O
ATOM  2415 N   GLU B 53     8.219  81.404  59.289  1.00 18.50    B   N
ATOM  2416 CA  GLU B 53     9.584  81.811  59.573  1.00 17.94    B   C
ATOM  2417 CB  GLU B 53    10.551  80.751  59.038  1.00 17.42    B   C
ATOM  2418 CG  GLU B 53    10.566  79.507  59.927  1.00 15.49    B   C
ATOM  2419 CD  GLU B 53    11.305  78.332  59.323  1.00 17.96    B   C
ATOM  2420 OE1 GLU B 53    12.087  78.534  58.374  1.00 18.58    B   O
ATOM  2421 OE2 GLU B 53    11.105  77.201  59.813  1.00 19.70    B   O
ATOM  2422 C   GLU B 53     9.897  83.193  59.005  1.00 18.71    B   C
ATOM  2423 O   GLU B 53    10.680  83.945  59.579  1.00 19.86    B   O
ATOM  2424 N   ALA B 54     9.271  83.537  57.885  1.00 18.53    B   N
ATOM  2425 CA  ALA B 54     9.492  84.848  57.283  1.00 16.14    B   C
ATOM  2426 CB  ALA B 54     8.744  84.951  55.954  1.00 13.28    B   C
ATOM  2427 C   ALA B 54     9.009  85.934  58.257  1.00 18.34    B   C
ATOM  2428 O   ALA B 54     9.636  86.987  58.393  1.00 16.94    B   O
ATOM  2429 N   LEU B 55     7.898  85.669  58.941  1.00 17.14    B   N
ATOM  2430 CA  LEU B 55     7.361  86.629  59.901  1.00 18.57    B   C
ATOM  2431 CB  LEU B 55     6.118  86.060  60.594  1.00 19.89    B   C
ATOM  2432 CG  LEU B 55     4.827  85.855  59.795  1.00 20.72    B   C
ATOM  2433 CD1 LEU B 55     3.771  85.221  60.706  1.00 22.99    B   C
ATOM  2434 CD2 LEU B 55     4.321  87.192  59.251  1.00 23.42    B   C
ATOM  2435 C   LEU B 55     8.405  86.999  60.956  1.00 18.71    B   C
ATOM  2436 O   LEU B 55     8.555  88.170  61.301  1.00 17.21    B   O
ATOM  2437 N   ASP B 56     9.131  86.002  61.458  1.00 18.83    B   N
ATOM  2438 CA  ASP B 56    10.151  86.241  62.474  1.00 18.36    B   C
ATOM  2439 CB  ASP B 56    10.829  84.924  62.881  1.00 21.45    B   C
ATOM  2440 CG  ASP B 56     9.875  83.958  63.581  1.00 24.57    B   C
ATOM  2441 OD1 ASP B 56     9.003  84.419  64.344  1.00 27.38    B   O
ATOM  2442 OD2 ASP B 56    10.005  82.729  63.383  1.00 26.87    B   O
ATOM  2443 C   ASP B 56    11.211  87.240  62.014  1.00 19.11    B   C
ATOM  2444 O   ASP B 56    11.669  88.082  62.792  1.00 17.72    B   O
ATOM  2445 N   PHE B 57    11.598  87.154  60.746  1.00 17.66    B   N
ATOM  2446 CA  PHE B 57    12.607  88.063  60.216  1.00 16.52    B   C
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Figure 7RR

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ATOM  2447 CB  PHE B  57    12.867  87.794  58.732  1.00 16.73    B   C
ATOM  2448 CG  PHE B  57    13.656  88.879  58.071  1.00 17.10    B   C
ATOM  2449 CD1 PHE B  57    15.035  88.958  58.247  1.00 19.76    B   C
ATOM  2450 CD2 PHE B  57    13.010  89.889  57.366  1.00 14.93    B   C
ATOM  2451 CE1 PHE B  57    15.759  90.031  57.738  1.00 19.78    B   C
ATOM  2452 CE2 PHE B  57    13.721  90.966  56.854  1.00 19.53    B   C
ATOM  2453 CZ  PHE B  57    15.100  91.039  57.041  1.00 19.60    B   C
ATOM  2454 C   PHE B  57    12.222  89.529  60.360  1.00 16.52    B   C
ATOM  2455 O   PHE B  57    13.057  90.365  60.699  1.00 18.03    B   O
ATOM  2456 N   PHE B  58    10.962  89.842  60.082  1.00 15.91    B   N
ATOM  2457 CA  PHE B  58    10.497  91.222  60.144  1.00 18.80    B   C
ATOM  2458 CB  PHE B  58     9.233  91.385  59.295  1.00 17.22    B   C
ATOM  2459 CG  PHE B  58     9.465  91.219  57.825  1.00 18.15    B   C
ATOM  2460 CD1 PHE B  58     9.217  90.004  57.199  1.00 18.00    B   C
ATOM  2461 CD2 PHE B  58     9.927  92.283  57.061  1.00 17.52    B   C
ATOM  2462 CE1 PHE B  58     9.423  89.852  55.831  1.00 16.31    B   C
ATOM  2463 CE2 PHE B  58    10.136  92.142  55.694  1.00 16.57    B   C
ATOM  2464 CZ  PHE B  58     9.884  90.924  55.077  1.00 17.04    B   C
ATOM  2465 C   PHE B  58    10.224  91.809  61.522  1.00 18.66    B   C
ATOM  2466 O   PHE B  58    10.140  93.028  61.662  1.00 21.14    B   O
ATOM  2467 N   LYS B  59    10.080  90.958  62.531  1.00 19.45    B   N
ATOM  2468 CA  LYS B  59     9.769  91.429  63.877  1.00 21.34    B   C
ATOM  2469 CB  LYS B  59     9.816  90.258  64.858  1.00 22.87    B   C
ATOM  2470 CG  LYS B  59     8.740  89.213  64.571  1.00 27.48    B   C
ATOM  2471 CD  LYS B  59     8.762  88.088  65.585  1.00 28.84    B   C
ATOM  2472 CE  LYS B  59     7.612  87.121  65.345  1.00 32.72    B   C
ATOM  2473 NZ  LYS B  59     6.308  87.829  65.430  1.00 35.68    B   N
ATOM  2474 C   LYS B  59    10.614  92.596  64.384  1.00 20.43    B   C
ATOM  2475 O   LYS B  59    10.073  93.621  64.792  1.00 19.96    B   O
ATOM  2476 N   PRO B  60    11.948  92.468  64.356  1.00 20.32    B   N
ATOM  2477 CD  PRO B  60    12.784  91.337  63.911  1.00 19.12    B   C
ATOM  2478 CA  PRO B  60    12.776  93.579  64.837  1.00 19.99    B   C
ATOM  2479 CB  PRO B  60    14.181  92.980  64.848  1.00 21.24    B   C
ATOM  2480 CG  PRO B  60    14.131  91.991  63.719  1.00 22.69    B   C
ATOM  2481 C   PRO B  60    12.690  94.859  63.995  1.00 20.53    B   C
ATOM  2482 O   PRO B  60    13.030  95.943  64.472  1.00 18.48    B   O
ATOM  2483 N   HIS B  61    12.221  94.740  62.756  1.00 18.92    B   N
ATOM  2484 CA  HIS B  61    12.116  95.896  61.871  1.00 20.35    B   C
ATOM  2485 CB  HIS B  61    12.099  95.433  60.413  1.00 19.99    B   C
ATOM  2486 CG  HIS B  61    13.409  94.875  59.953  1.00 19.89    B   C
ATOM  2487 CD2 HIS B  61    13.820  93.599  59.768  1.00 21.62    B   C
ATOM  2488 ND1 HIS B  61    14.499  95.673  59.678  1.00 21.05    B   N
ATOM  2489 CE1 HIS B  61    15.526  94.912  59.343  1.00 22.27    B   C
ATOM  2490 NE2 HIS B  61    15.142  93.649  59.390  1.00 21.05    B   N
ATOM  2491 C   HIS B  61    10.904  96.770  62.170  1.00 21.73    B   C
ATOM  2492 O   HIS B  61    10.808  97.899  61.691  1.00 22.05    B   O
ATOM  2493 N   GLU B  62     9.985  96.242  62.969  1.00 21.87    B   N
ATOM  2494 CA  GLU B  62     8.792  96.982  63.354  1.00 23.56    B   C
ATOM  2495 CB  GLU B  62     9.181  98.106  64.318  1.00 24.92    B   C
ATOM  2496 CG  GLU B  62    10.003  97.606  65.496  1.00 30.01    B   C
ATOM  2497 CD  GLU B  62    10.361  98.699  66.481  1.00 33.69    B   C
ATOM  2498 OE1 GLU B  62    10.896  99.743  66.053  1.00 35.60    B   O
ATOM  2499 OE2 GLU B  62    10.116  98.505  67.688  1.00 36.17    B   O
ATOM  2500 C   GLU B  62     8.044  97.552  62.157  1.00 22.92    B   C
ATOM  2501 O   GLU B  62     7.701  98.739  62.126  1.00 21.97    B   O
ATOM  2502 N   ILE B  63     7.795  96.706  61.164  1.00 19.69    B   N
ATOM  2503 CA  ILE B  63     7.064  97.144  59.987  1.00 18.17    B   C
ATOM  2504 CB  ILE B  63     7.236  96.149  58.825  1.00 17.22    B   C
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Figure 7SS

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ATOM  2505 CG2 ILE B  63      8.686  96.146  58.370  1.00 15.56      B   C
ATOM  2506 CG1 ILE B  63      6.817  94.746  59.269  1.00 15.21      B   C
ATOM  2507 CD1 ILE B  63.     6.745  93.736  58.131  1.00 15.19      B   C
ATOM  2508 C   ILE B  63      5.590  97.258  60.375  1.00 18.21      B   C
ATOM  2509 O   ILE B  63      5.127  96.575  61.294  1.00 17.53      B   O
ATOM  2510 N   GLU B  64      4.859  98.125  59.683  1.00 16.97      B   N
ATOM  2511 CA  GLU B  64      3.445  98.349  59.985  1.00 17.61      B   C
ATOM  2512 CB  GLU B  64      3.089  99.813  59.718  1.00 18.92      B   C
ATOM  2513 CG  GLU B  64      3.934 100.801  60.499  1.00 23.07      B   C
ATOM  2514 CD  GLU B  64      3.697 102.235  60.067  1.00 26.42      B   C
ATOM  2515 OE1 GLU B  64      2.541 102.702  60.167  1.00 28.70      B   O
ATOM  2516 OE2 GLU B  64      4.667 102.889  59.624  1.00 25.35      B   O
ATOM  2517 C   GLU B  64      2.511  97.452  59.187  1.00 16.83      B   C
ATOM  2518 O   GLU B  64      1.349  97.259  59.548  1.00 16.07      B   O
ATOM  2519 N   LEU B  65      3.035  96.896  58.104  1.00 17.77      B   N
ATOM  2520 CA  LEU B  65      2.261  96.031  57.232  1.00 16.43      B   C
ATOM  2521 CB  LEU B  65      1.398  96.895  56.302  1.00 18.09      B   C
ATOM  2522 CG  LEU B  65      0.640  96.266  55.133  1.00 21.97      B   C
ATOM  2523 CD1 LEU B  65     -0.529  97.164  54.757  1.00 21.04      B   C
ATOM  2524 CD2 LEU B  65      1.572  96.066  53.944  1.00 20.71      B   C
ATOM  2525 C   LEU B  65      3.244  95.195  56.430  1.00 14.51      B   C
ATOM  2526 O   LEU B  65      4.345  95.648  56.123  1.00 12.92      B   O
ATOM  2527 N   LEU B  66      2.853  93.971  56.102  1.00 14.75      B   N
ATOM  2528 CA  LEU B  66      3.722  93.092  55.329  1.00 14.89      B   C
ATOM  2529 CB  LEU B  66      4.020  91.810  56.110  1.00 14.10      B   C
ATOM  2530 CG  LEU B  66      4.753  90.716  55.326  1.00 16.87      B   C
ATOM  2531 CD1 LEU B  66      6.149  91.214  54.949  1.00 16.67      B   C
ATOM  2532 CD2 LEU B  66      4.844  89.433  56.169  1.00 17.63      B   C
ATOM  2533 C   LEU B  66      3.091  92.722  53.995  1.00 14.55      B   C
ATOM  2534 O   LEU B  66      1.911  92.374  53.923  1.00 16.90      B   O
ATOM  2535 N   ILE B  67      3.884  92.813  52.937  1.00 14.59      B   N
ATOM  2536 CA  ILE B  67      3.422  92.451  51.610  1.00 14.92      B   C
ATOM  2537 CB  ILE B  67      3.775  93.524  50.560  1.00 17.24      B   C
ATOM  2538 CG2 ILE B  67      3.458  93.000  49.150  1.00 14.44      B   C
ATOM  2539 CG1 ILE B  67      2.995  94.815  50.846  1.00 17.41      B   C
ATOM  2540 CD1 ILE B  67      3.287  95.933  49.859  1.00 18.39      B   C
ATOM  2541 C   ILE B  67      4.117  91.159  51.207  1.00 13.22      B   C
ATOM  2542 O   ILE B  67      5.344  91.077  51.219  1.00 13.66      B   O
ATOM  2543 N   VAL B  68      3.330  90.144  50.875  1.00 13.61      B   N
ATOM  2544 CA  VAL B  68      3.898  88.878  50.430  1.00 13.77      B   C
ATOM  2545 CB  VAL B  68      3.065  87.683  50.915  1.00 12.35      B   C
ATOM  2546 CG1 VAL B  68      3.692  86.381  50.426  1.00 10.26      B   C
ATOM  2547 CG2 VAL B  68      2.991  87.699  52.438  1.00 12.86      B   C
ATOM  2548 C   VAL B  68      3.865  88.950  48.907  1.00 12.64      B   C
ATOM  2549 O   VAL B  68      2.839  88.673  48.283  1.00 14.77      B   O
ATOM  2550 N   ALA B  69      4.988  89.349  48.319  1.00 12.26      B   N
ATOM  2551 CA  ALA B  69      5.101  89.499  46.870  1.00 10.06      B   C
ATOM  2552 CB  ALA B  69      6.412  90.194  46.529  1.00  9.84      B   C
ATOM  2553 C   ALA B  69      5.027  88.163  46.147  1.00 12.35      B   C
ATOM  2554 O   ALA B  69      4.635  88.096  44.980  1.00  9.71      B   O
ATOM  2555 N   CYS B  70      5.427  87.104  46.844  1.00 11.11      B   N
ATOM  2556 CA  CYS B  70      5.418  85.766  46.273  1.00 11.24      B   C
ATOM  2557 CB  CYS B  70      6.207  84.816  47.176  1.00 11.62      B   C
ATOM  2558 SG  CYS B  70      6.347  83.142  46.504  1.00 12.64      B   S
ATOM  2559 C   CYS B  70      4.001  85.229  46.070  1.00 11.05      B   C
ATOM  2560 O   CYS B  70      3.205  85.177  47.010  1.00 11.37      B   O
ATOM  2561 N   ASN B  71      3.688  84.823  44.840  1.00 12.49      B   N
ATOM  2562 CA  ASN B  71      2.365  84.279  44.543  1.00 11.50      B   C
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Figure 7TT

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ATOM  2563 CB  ASN B  71      2.157  84.145  43.031  1.00  9.14      B   C
ATOM  2564 CG  ASN B  71      2.258  85.471  42.306  1.00 11.76      B   C
ATOM  2565 OD1 ASN B  71      3.344  86.024  42.151  1.00 10.78      B   O
ATOM  2566 ND2 ASN B  71      1.117  85.996  41.867  1.00 11.54      B   N
ATOM  2567 C   ASN B  71      2.192  82.909  45.186  1.00 12.35      B   C
ATOM  2568 O   ASN B  71      1.078  82.526  45.575  1.00  8.22      B   O
ATOM  2569 N   THR B  72      3.292  82.164  45.270  1.00 11.41      B   N
ATOM  2570 CA  THR B  72      3.257  80.831  45.863  1.00 12.16      B   C
ATOM  2571 CB  THR B  72      4.572  80.062  45.611  1.00 13.52      B   C
ATOM  2572 OG1 THR B  72      4.704  79.791  44.212  1.00 14.69      B   O
ATOM  2573 CG2 THR B  72      4.581  78.741  46.380  1.00 11.87      B   C
ATOM  2574 C   THR B  72      3.012  80.915  47.357  1.00 12.59      B   C
ATOM  2575 O   THR B  72      2.166  80.200  47.892  1.00 14.73      B   O
ATOM  2576 N   ALA B  73      3.754  81.784  48.034  1.00 13.02      B   N
ATOM  2577 CA  ALA B  73      3.576  81.953  49.471  1.00 13.51      B   C
ATOM  2578 CB  ALA B  73      4.676  82.830  50.044  1.00 13.14      B   C
ATOM  2579 C   ALA B  73      2.206  82.571  49.739  1.00 13.74      B   C
ATOM  2580 O   ALA B  73      1.580  82.278  50.752  1.00 12.89      B   O
ATOM  2581 N   SER B  74      1.751  83.437  48.830  1.00 14.66      B   N
ATOM  2582 CA  SER B  74      0.439  84.066  48.967  1.00 14.25      B   C
ATOM  2583 CB  SER B  74      0.212  85.099  47.853  1.00 13.54      B   C
ATOM  2584 OG  SER B  74      0.996  86.268  48.040  1.00 13.45      B   O
ATOM  2585 C   SER B  74     -0.655  83.002  48.877  1.00 16.32      B   C
ATOM  2586 O   SER B  74     -1.668  83.065  49.575  1.00 14.08      B   O
ATOM  2587 N   ALA B  75     -0.443  82.028  48.002  1.00 16.22      B   N
ATOM  2588 CA  ALA B  75     -1.416  80.966  47.797  1.00 17.85      B   C
ATOM  2589 CB  ALA B  75     -1.170  80.291  46.449  1.00 18.98      B   C
ATOM  2590 C   ALA B  75     -1.438  79.911  48.890  1.00 18.56      B   C
ATOM  2591 O   ALA B  75     -2.498  79.377  49.217  1.00 19.22      B   O
ATOM  2592 N   LEU B  76     -0.274  79.608  49.455  1.00 17.86      B   N
ATOM  2593 CA  LEU B  76     -0.196  78.570  50.473  1.00 19.90      B   C
ATOM  2594 CB  LEU B  76      0.921  77.580  50.131  1.00 19.60      B   C
ATOM  2595 CG  LEU B  76      0.703  76.565  49.004  1.00 21.94      B   C
ATOM  2596 CD1 LEU B  76     -0.579  75.764  49.283  1.00 19.11      B   C
ATOM  2597 CD2 LEU B  76      0.610  77.284  47.670  1.00 23.22      B   C
ATOM  2598 C   LEU B  76     -0.021  78.978  51.925  1.00 19.97      B   C
ATOM  2599 O   LEU B  76     -0.643  78.388  52.800  1.00 19.54      B   O
ATOM  2600 N   ALA B  77      0.815  79.980  52.183  1.00 20.55      B   N
ATOM  2601 CA  ALA B  77      1.111  80.380  53.559  1.00 22.00      B   C
ATOM  2602 CB  ALA B  77      2.616  80.581  53.700  1.00 20.40      B   C
ATOM  2603 C   ALA B  77      0.392  81.590  54.149  1.00 21.97      B   C
ATOM  2604 O   ALA B  77      0.420  81.792  55.365  1.00 17.66      B   O
ATOM  2605 N   LEU B  78     -0.247  82.386  53.299  1.00 23.46      B   N
ATOM  2606 CA  LEU B  78     -0.916  83.595  53.757  1.00 24.17      B   C
ATOM  2607 CB  LEU B  78     -1.634  84.271  52.583  1.00 23.46      B   C
ATOM  2608 CG  LEU B  78     -2.166  85.692  52.799  1.00 24.62      B   C
ATOM  2609 CD1 LEU B  78     -1.042  86.612  53.256  1.00 25.18      B   C
ATOM  2610 CD2 LEU B  78     -2.770  86.204  51.499  1.00 21.11      B   C
ATOM  2611 C   LEU B  78     -1.885  83.387  54.918  1.00 23.63      B   C
ATOM  2612 O   LEU B  78     -1.820  84.098  55.918  1.00 20.90      B   O
ATOM  2613 N   GLU B  79     -2.775  82.410  54.798  1.00 24.20      B   N
ATOM  2614 CA  GLU B  79     -3.744  82.171  55.856  1.00 25.27      B   C
ATOM  2615 CB  GLU B  79     -4.643  80.987  55.496  1.00 27.94      B   C
ATOM  2616 CG  GLU B  79     -5.845  80.830  56.417  1.00 34.09      B   C
ATOM  2617 CD  GLU B  79     -6.760  79.694  55.997  1.00 36.98      B   C
ATOM  2618 OE1 GLU B  79     -7.246  79.714  54.847  1.00 38.97      B   O
ATOM  2619 OE2 GLU B  79     -6.994  78.781  56.818  1.00 40.71      B   O
ATOM  2620 C   GLU B  79     -3.066  81.921  57.199  1.00 24.66      B   C
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Figure 7UU

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ATOM  2621 O   GLU B 79    -3.434  82.519  58.208  1.00 21.76    B   O
ATOM  2622 N   GLU B 80    -2.063  81.050  57.213  1.00 25.11    B   N
ATOM  2623 CA  GLU B 80    -1.367  80.740  58.455  1.00 25.16    B   C
ATOM  2624 CB  GLU B 80    -0.425  79.549  58.249  1.00 30.59    B   C
ATOM  2625 CG  GLU B 80    -0.324  78.632  59.464  1.00 36.68    B   C
ATOM  2626 CD  GLU B 80    -1.674  78.055  59.876  1.00 39.61    B   C
ATOM  2627 OE1 GLU B 80    -2.275  77.297  59.085  1.00 42.54    B   O
ATOM  2628 OE2 GLU B 80    -2.139  78.363  60.993  1.00 41.38    B   O
ATOM  2629 C   GLU B 80    -0.587  81.942  58.987  1.00 24.73    B   C
ATOM  2630 O   GLU B 80    -0.590  82.211  60.190  1.00 24.93    B   O
ATOM  2631 N   MET B 81     0.072  82.670  58.092  1.00 22.49    B   N
ATOM  2632 CA  MET B 81     0.851  83.838  58.492  1.00 20.82    B   C
ATOM  2633 CB  MET B 81     1.559  84.437  57.275  1.00 18.38    B   C
ATOM  2634 CG  MET B 81     2.671  83.563  56.717  1.00 18.17    B   C
ATOM  2635 SD  MET B 81     3.255  84.147  55.112  1.00 17.68    B   S
ATOM  2636 CE  MET B 81     4.308  85.481  55.573  1.00 12.45    B   C
ATOM  2637 C   MET B 81    -0.015  84.907  59.155  1.00 20.81    B   C
ATOM  2638 O   MET B 81     0.382  85.508  60.154  1.00 19.23    B   O
ATOM  2639 N   GLN B 82    -1.193  85.145  58.589  1.00 20.82    B   N
ATOM  2640 CA  GLN B 82    -2.111  86.145  59.129  1.00 22.97    B   C
ATOM  2641 CB  GLN B 82    -3.286  86.367  58.168  1.00 23.14    B   C
ATOM  2642 CG  GLN B 82    -2.861  86.867  56.787  1.00 22.68    B   C
ATOM  2643 CD  GLN B 82    -4.024  87.016  55.821  1.00 25.48    B   C
ATOM  2644 OE1 GLN B 82    -4.830  86.097  55.650  1.00 24.87    B   O
ATOM  2645 NE2 GLN B 82    -4.110  88.175  55.172  1.00 25.37    B   N
ATOM  2646 C   GLN B 82    -2.627  85.695  60.482  1.00 22.69    B   C
ATOM  2647 O   GLN B 82    -2.905  86.514  61.357  1.00 22.32    B   O
ATOM  2648 N   LYS B 83    -2.752  84.387  60.656  1.00 24.09    B   N
ATOM  2649 CA  LYS B 83    -3.235  83.851  61.918  1.00 25.60    B   C
ATOM  2650 CB  LYS B 83    -3.376  82.328  61.829  1.00 27.86    B   C
ATOM  2651 CG  LYS B 83    -3.766  81.658  63.141  1.00 32.07    B   C
ATOM  2652 CD  LYS B 83    -3.799  80.148  62.990  1.00 33.64    B   C
ATOM  2653 CE  LYS B 83    -4.118  79.453  64.308  1.00 38.06    B   C
ATOM  2654 NZ  LYS B 83    -4.127  77.965  64.142  1.00 38.15    B   N
ATOM  2655 C   LYS B 83    -2.298  84.218  63.065  1.00 25.66    B   C
ATOM  2656 O   LYS B 83    -2.750  84.586  64.149  1.00 23.94    B   O
ATOM  2657 N   TYR B 84    -0.993  84.134  62.825  1.00 25.08    B   N
ATOM  2658 CA  TYR B 84    -0.022  84.442  63.870  1.00 24.54    B   C
ATOM  2659 CB  TYR B 84     1.063  83.367  63.913  1.00 27.22    B   C
ATOM  2660 CG  TYR B 84     0.542  81.986  64.219  1.00 30.76    B   C
ATOM  2661 CD1 TYR B 84     0.162  81.119  63.195  1.00 31.28    B   C
ATOM  2662 CE1 TYR B 84    -0.325  79.844  63.476  1.00 34.59    B   C
ATOM  2663 CD2 TYR B 84     0.421  81.546  65.538  1.00 32.96    B   C
ATOM  2664 CE2 TYR B 84    -0.066  80.276  65.832  1.00 35.61    B   C
ATOM  2665 CZ  TYR B 84    -0.435  79.430  64.797  1.00 36.06    B   C
ATOM  2666 OH  TYR B 84    -0.904  78.167  65.089  1.00 37.33    B   O
ATOM  2667 C   TYR B 84     0.641  85.808  63.764  1.00 23.89    B   C
ATOM  2668 O   TYR B 84     1.704  86.030  64.341  1.00 25.50    B   O
ATOM  2669 N   SER B 85     0.014  86.726  63.040  1.00 22.10    B   N
ATOM  2670 CA  SER B 85     0.563  88.067  62.874  1.00 21.74    B   C
ATOM  2671 CB  SER B 85     0.884  88.323  61.397  1.00 19.79    B   C
ATOM  2672 OG  SER B 85     1.259  89.673  61.181  1.00 25.60    B   O
ATOM  2673 C   SER B 85    -0.413  89.127  63.374  1.00 21.62    B   C
ATOM  2674 O   SER B 85    -1.621  89.009  63.177  1.00 21.34    B   O
ATOM  2675 N   LYS B 86     0.107  90.157  64.031  1.00 20.33    B   N
ATOM  2676 CA  LYS B 86    -0.750  91.221  64.519  1.00 22.30    B   C
ATOM  2677 CB  LYS B 86    -0.235  91.776  65.853  1.00 25.37    B   C
ATOM  2678 CG  LYS B 86     1.182  92.304  65.826  1.00 31.07    B   C
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Figure 7VV

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ATOM  2679 CD  LYS B 86     1.629  92.685  67.231  1.00 35.40    B   C
ATOM  2680 CE  LYS B 86     1.562  91.486  68.175  1.00 35.66    B   C
ATOM  2681 NZ  LYS B 86     1.952  91.849  69.565  1.00 39.76    B   N
ATOM  2682 C   LYS B 86    -0.860  92.333  63.482  1.00 22.13    B   C
ATOM  2683 O   LYS B 86    -1.871  93.028  63.433  1.00 23.41    B   O
ATOM  2684 N   ILE B 87     0.169  92.499  62.649  1.00 20.24    B   N
ATOM  2685 CA  ILE B 87     0.127  93.524  61.605  1.00 18.31    B   C
ATOM  2686 CB  ILE B 87     1.543  94.004  61.181  1.00 16.92    B   C
ATOM  2687 CG2 ILE B 87     2.244  94.688  62.359  1.00 18.70    B   C
ATOM  2688 CG1 ILE B 87     2.361  92.822  60.650  1.00 17.63    B   C
ATOM  2689 CD1 ILE B 87     3.721  93.203  60.117  1.00 17.00    B   C
ATOM  2690 C   ILE B 87    -0.559  92.921  60.384  1.00 17.72    B   C
ATOM  2691 O   ILE B 87    -0.553  91.707  60.193  1.00 18.08    B   O
ATOM  2692 N   PRO B 88    -1.173  93.762  59.542  1.00 18.77    B   N
ATOM  2693 CD  PRO B 88    -1.340  95.223  59.619  1.00 17.15    B   C
ATOM  2694 CA  PRO B 88    -1.839  93.216  58.358  1.00 19.35    B   C
ATOM  2695 CB  PRO B 88    -2.575  94.428  57.789  1.00 20.10    B   C
ATOM  2696 CG  PRO B 88    -1.691  95.572  58.194  1.00 21.95    B   C
ATOM  2697 C   PRO B 88    -0.844  92.619  57.360  1.00 18.71    B   C
ATOM  2698 O   PRO B 88     0.247  93.148  57.163  1.00 18.85    B   O
ATOM  2699 N   ILE B 89    -1.222  91.498  56.759  1.00 17.91    B   N
ATOM  2700 CA  ILE B 89    -0.387  90.848  55.757  1.00 17.91    B   C
ATOM  2701 CB  ILE B 89    -0.011  89.404  56.164  1.00 18.44    B   C
ATOM  2702 CG2 ILE B 89     0.952  88.807  55.133  1.00 18.14    B   C
ATOM  2703 CG1 ILE B 89     0.658  89.408  57.543  1.00 21.01    B   C
ATOM  2704 CD1 ILE B 89     1.125  88.043  58.007  1.00 18.58    B   C
ATOM  2705 C   ILE B 89    -1.202  90.823  54.466  1.00 17.23    B   C
ATOM  2706 O   ILE B 89    -2.323  90.305  54.425  1.00 17.75    B   O
ATOM  2707 N   VAL B 90    -0.642  91.403  53.414  1.00 16.10    B   N
ATOM  2708 CA  VAL B 90    -1.334  91.467  52.141  1.00 15.66    B   C
ATOM  2709 CB  VAL B 90    -1.436  92.934  51.651  1.00 17.82    B   C
ATOM  2710 CG1 VAL B 90    -2.241  93.001  50.351  1.00 17.58    B   C
ATOM  2711 CG2 VAL B 90    -2.074  93.805  52.739  1.00 18.13    B   C
ATOM  2712 C   VAL B 90    -0.612  90.640  51.088  1.00 13.43    B   C
ATOM  2713 O   VAL B 90     0.567  90.869  50.812  1.00 14.69    B   O
ATOM  2714 N   GLY B 91    -1.332  89.681  50.511  1.00 13.52    B   N
ATOM  2715 CA  GLY B 91    -0.773  88.827  49.474  1.00 12.39    B   C
ATOM  2716 C   GLY B 91    -1.085  89.387  48.093  1.00 14.87    B   C
ATOM  2717 O   GLY B 91    -1.754  90.414  47.982  1.00 13.52    B   O
ATOM  2718 N   VAL B 92    -0.618  88.715  47.041  1.00 13.75    B   N
ATOM  2719 CA  VAL B 92    -0.840  89.190  45.676  1.00 14.98    B   C
ATOM  2720 CB  VAL B 92     0.447  89.066  44.819  1.00 14.03    B   C
ATOM  2721 CG1 VAL B 92     1.442  90.130  45.234  1.00  9.89    B   C
ATOM  2722 CG2 VAL B 92     1.056  87.672  44.978  1.00 12.60    B   C
ATOM  2723 C   VAL B 92    -1.975  88.505  44.922  1.00 16.65    B   C
ATOM  2724 O   VAL B 92    -2.194  88.786  43.746  1.00 17.87    B   O
ATOM  2725 N   ILE B 93    -2.702  87.616  45.585  1.00 16.90    B   N
ATOM  2726 CA  ILE B 93    -3.798  86.933  44.909  1.00 17.60    B   C
ATOM  2727 CB  ILE B 93    -3.993  85.514  45.469  1.00 18.08    B   C
ATOM  2728 CG2 ILE B 93    -5.148  84.825  44.757  1.00 15.25    B   C
ATOM  2729 CG1 ILE B 93    -2.693  84.722  45.291  1.00 18.10    B   C
ATOM  2730 CD1 ILE B 93    -2.803  83.256  45.609  1.00 20.71    B   C
ATOM  2731 C   ILE B 93    -5.125  87.693  44.971  1.00 18.37    B   C
ATOM  2732 O   ILE B 93    -5.720  87.983  43.930  1.00 19.27    B   O
ATOM  2733 N   GLU B 94    -5.590  88.021  46.176  1.00 18.78    B   N
ATOM  2734 CA  GLU B 94    -6.859  88.742  46.315  1.00 21.11    B   C
ATOM  2735 CB  GLU B 94    -7.198  88.977  47.789  1.00 23.95    B   C
ATOM  2736 CG  GLU B 94    -7.565  87.705  48.536  1.00 28.58    B   C
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Figure 7WW

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ATOM  2737 CD  GLU B  94     -8.651  86.906  47.831  1.00 33.34      B   C
ATOM  2738 OE1 GLU B  94     -9.700  87.494  47.484  1.00 32.87      B   O
ATOM  2739 OE2 GLU B  94     -8.453  85.686  47.627  1.00 36.08      B   O
ATOM  2740 C   GLU B  94     -6.873  90.073  45.568  1.00 20.94      B   C
ATOM  2741 O   GLU B  94     -7.882  90.439  44.960  1.00 21.06      B   O
ATOM  2742 N   PRO B  95     -5.760  90.823  45.615  1.00 19.29      B   N
ATOM  2743 CD  PRO B  95     -4.581  90.667  46.487  1.00 17.34      B   C
ATOM  2744 CA  PRO B  95     -5.714  92.108  44.909  1.00 19.84      B   C
ATOM  2745 CB  PRO B  95     -4.301  92.603  45.196  1.00 18.81      B   C
ATOM  2746 CG  PRO B  95     -4.058  92.087  46.580  1.00 19.00      B   C
ATOM  2747 C   PRO B  95     -5.971  91.933  43.415  1.00 18.63      B   C
ATOM  2748 O   PRO B  95     -6.588  92.786  42.771  1.00 19.30      B   O
ATOM  2749 N   SER B  96     -5.485  90.824  42.867  1.00 20.23      B   N
ATOM  2750 CA  SER B  96     -5.661  90.532  41.451  1.00 19.54      B   C
ATOM  2751 CB  SER B  96     -4.752  89.380  41.032  1.00 20.19      B   C
ATOM  2752 OG  SER B  96     -3.398  89.803  41.022  1.00 21.10      B   O
ATOM  2753 C   SER B  96     -7.107  90.194  41.137  1.00 19.82      B   C
ATOM  2754 O   SER B  96     -7.623  90.554  40.076  1.00 18.36      B   O
ATOM  2755 N   ILE B  97     -7.761  89.496  42.060  1.00 19.40      B   N
ATOM  2756 CA  ILE B  97     -9.159  89.129  41.869  1.00 21.46      B   C
ATOM  2757 CB  ILE B  97     -9.702  88.310  43.066  1.00 20.75      B   C
ATOM  2758 CG2 ILE B  97    -11.185  88.032  42.872  1.00 23.74      B   C
ATOM  2759 CG1 ILE B  97     -8.929  86.996  43.205  1.00 20.33      B   C
ATOM  2760 CD1 ILE B  97     -9.130  86.028  42.048  1.00 18.39      B   C
ATOM  2761 C   ILE B  97     -9.985  90.408  41.741  1.00 20.42      B   C
ATOM  2762 O   ILE B  97    -10.881  90.502  40.904  1.00 21.88      B   O
ATOM  2763 N   LEU B  98     -9.670  91.393  42.575  1.00 22.89      B   N
ATOM  2764 CA  LEU B  98    -10.378  92.668  42.561  1.00 22.94      B   C
ATOM  2765 CB  LEU B  98     -9.918  93.539  43.734  1.00 24.42      B   C
ATOM  2766 CG  LEU B  98    -10.197  92.998  45.143  1.00 24.87      B   C
ATOM  2767 CD1 LEU B  98     -9.532  93.893  46.172  1.00 27.53      B   C
ATOM  2768 CD2 LEU B  98    -11.701  92.922  45.389  1.00 25.92      B   C
ATOM  2769 C   LEU B  98    -10.150  93.411  41.249  1.00 23.55      B   C
ATOM  2770 O   LEU B  98    -11.067  94.032  40.708  1.00 24.17      B   O
ATOM  2771 N   ALA B  99     -8.924  93.351  40.740  1.00 23.11      B   N
ATOM  2772 CA  ALA B  99     -8.594  94.025  39.491  1.00 22.89      B   C
ATOM  2773 CB  ALA B  99     -7.110  93.904  39.208  1.00 22.27      B   C
ATOM  2774 C   ALA B  99     -9.390  93.395  38.362  1.00 21.70      B   C
ATOM  2775 O   ALA B  99     -9.921  94.090  37.497  1.00 18.65      B   O
ATOM  2776 N   ILE B 100     -9.457  92.068  38.377  1.00 19.64      B   N
ATOM  2777 CA  ILE B 100    -10.190  91.331  37.363  1.00 19.82      B   C
ATOM  2778 CB  ILE B 100    -10.044  89.803  37.568  1.00 21.33      B   C
ATOM  2779 CG2 ILE B 100    -11.118  89.054  36.784  1.00 19.75      B   C
ATOM  2780 CG1 ILE B 100     -8.644  89.357  37.134  1.00 20.47      B   C
ATOM  2781 CD1 ILE B 100     -8.425  87.859  37.227  1.00 23.03      B   C
ATOM  2782 C   ILE B 100    -11.664  91.717  37.413  1.00 20.18      B   C
ATOM  2783 O   ILE B 100    -12.310  91.842  36.378  1.00 17.92      B   O
ATOM  2784 N   LYS B 101    -12.192  91.910  38.617  1.00 21.96      B   N
ATOM  2785 CA  LYS B 101    -13.594  92.296  38.755  1.00 24.71      B   C
ATOM  2786 CB  LYS B 101    -13.980  92.434  40.229  1.00 25.47      B   C
ATOM  2787 CG  LYS B 101    -14.034  91.120  40.988  1.00 30.47      B   C
ATOM  2788 CD  LYS B 101    -14.348  91.358  42.460  1.00 36.47      B   C
ATOM  2789 CE  LYS B 101    -15.720  91.992  42.654  1.00 39.30      B   C
ATOM  2790 NZ  LYS B 101    -15.973  92.336  44.087  1.00 42.89      B   N
ATOM  2791 C   LYS B 101    -13.831  93.623  38.041  1.00 24.26      B   C
ATOM  2792 O   LYS B 101    -14.846  93.797  37.369  1.00 25.28      B   O
ATOM  2793 N   ARG B 102    -12.886  94.548  38.185  1.00 23.53      B   N
ATOM  2794 CA  ARG B 102    -12.986  95.865  37.559  1.00 24.45      B   C
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Figure 7XX

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ATOM  2795  CB  ARG B 102    -11.976  96.835  38.182  1.00 24.23      B   C
ATOM  2796  CG  ARG B 102    -12.234  97.217  39.625  1.00 25.40      B   C
ATOM  2797  CD  ARG B 102    -11.276  98.316  40.054  1.00 26.37      B   C
ATOM  2798  NE  ARG B 102     -9.888  97.863  40.086  1.00 27.81      B   N
ATOM  2799  CZ  ARG B 102     -9.328  97.229  41.114  1.00 27.91      B   C
ATOM  2800  NH1 ARG B 102    -10.035  96.972  42.206  1.00 27.77      B   N
ATOM  2801  NH2 ARG B 102     -8.058  96.857  41.051  1.00 22.49      B   N
ATOM  2802  C   ARG B 102    -12.747  95.846  36.051  1.00 23.56      B   C
ATOM  2803  O   ARG B 102    -13.394  96.576  35.306  1.00 21.65      B   O
ATOM  2804  N   GLN B 103    -11.816  95.010  35.605  1.00 22.46      B   N
ATOM  2805  CA  GLN B 103    -11.474  94.951  34.189  1.00 22.58      B   C
ATOM  2806  CB  GLN B 103     -9.972  94.728  34.036  1.00 21.32      B   C
ATOM  2807  CG  GLN B 103     -9.126  95.766  34.733  1.00 22.61      B   C
ATOM  2808  CD  GLN B 103     -7.659  95.405  34.712  1.00 22.94      B   C
ATOM  2809  OE1 GLN B 103     -7.074  95.216  33.647  1.00 24.42      B   O
ATOM  2810  NE2 GLN B 103     -7.055  95.305  35.890  1.00 22.74      B   N
ATOM  2811  C   GLN B 103    -12.206  93.918  33.349  1.00 22.98      B   C
ATOM  2812  O   GLN B 103    -12.221  94.020  32.126  1.00 23.73      B   O
ATOM  2813  N   VAL B 104    -12.807  92.925  33.989  1.00 22.89      B   N
ATOM  2814  CA  VAL B 104    -13.500  91.881  33.241  1.00 24.65      B   C
ATOM  2815  CB  VAL B 104    -12.796  90.518  33.427  1.00 25.96      B   C
ATOM  2816  CG1 VAL B 104    -13.465  89.462  32.568  1.00 25.99      B   C
ATOM  2817  CG2 VAL B 104    -11.321  90.643  33.066  1.00 24.05      B   C
ATOM  2818  C   VAL B 104    -14.957  91.752  33.663  1.00 26.14      B   C
ATOM  2819  O   VAL B 104    -15.284  90.975  34.557  1.00 23.04      B   O
ATOM  2820  N   GLU B 105    -15.821  92.515  33.000  1.00 28.13      B   N
ATOM  2821  CA  GLU B 105    -17.253  92.520  33.289  1.00 31.78      B   C
ATOM  2822  CB  GLU B 105    -17.923  93.703  32.581  1.00 37.19      B   C
ATOM  2823  CG  GLU B 105    -17.318  95.053  32.940  1.00 47.02      B   C
ATOM  2824  CD  GLU B 105    -17.983  96.226  32.231  1.00 50.74      B   C
ATOM  2825  OE1 GLU B 105    -18.016  96.247  30.979  1.00 51.99      B   O
ATOM  2826  OE2 GLU B 105    -18.469  97.136  32.933  1.00 54.70      B   O
ATOM  2827  C   GLU B 105    -17.953  91.231  32.877  1.00 29.48      B   C
ATOM  2828  O   GLU B 105    -18.915  90.807  33.518  1.00 32.30      B   O
ATOM  2829  N   ASP B 106    -17.471  90.608  31.808  1.00 27.12      B   N
ATOM  2830  CA  ASP B 106    -18.067  89.377  31.310  1.00 26.01      B   C
ATOM  2831  CB  ASP B 106    -17.666  89.167  29.850  1.00 26.98      B   C
ATOM  2832  CG  ASP B 106    -18.215  87.881  29.272  1.00 28.23      B   C
ATOM  2833  OD1 ASP B 106    -19.054  87.232  29.930  1.00 28.83      B   O
ATOM  2834  OD2 ASP B 106    -17.807  87.521  28.147  1.00 31.85      B   O
ATOM  2835  C   ASP B 106    -17.666  88.168  32.147  1.00 25.85      B   C
ATOM  2836  O   ASP B 106    -16.517  87.736  32.118  1.00 24.84      B   O
ATOM  2837  N   LYS B 107    -18.628  87.626  32.890  1.00 25.49      B   N
ATOM  2838  CA  LYS B 107    -18.396  86.472  33.754  1.00 27.31      B   C
ATOM  2839  CB  LYS B 107    -19.633  86.210  34.622  1.00 29.26      B   C
ATOM  2840  CG  LYS B 107    -19.948  87.328  35.600  1.00 32.01      B   C
ATOM  2841  CD  LYS B 107    -18.757  87.611  36.512  1.00 33.91      B   C
ATOM  2842  CE  LYS B 107    -19.056  88.718  37.516  1.00 34.29      B   C
ATOM  2843  NZ  LYS B 107    -19.369  90.016  36.853  1.00 41.19      B   N
ATOM  2844  C   LYS B 107    -18.044  85.203  32.991  1.00 26.67      B   C
ATOM  2845  O   LYS B 107    -17.508  84.254  33.565  1.00 28.78      B   O
ATOM  2846  N   ASN B 108    -18.337  85.187  31.698  1.00 26.36      B   N
ATOM  2847  CA  ASN B 108    -18.059  84.019  30.875  1.00 27.30      B   C
ATOM  2848  CB  ASN B 108    -19.176  83.833  29.848  1.00 32.21      B   C
ATOM  2849  CG  ASN B 108    -20.509  83.515  30.496  1.00 37.21      B   C
ATOM  2850  OD1 ASN B 108    -20.670  82.470  31.130  1.00 41.66      B   O
ATOM  2851  ND2 ASN B 108    -21.473  84.420  30.350  1.00 39.88      B   N
ATOM  2852  C   ASN B 108    -16.719  84.106  30.160  1.00 25.00      B   C
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Figure 7YY

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ATOM  2853  O   ASN B 108    -16.318  83.173  29.467  1.00 27.12    B   O
ATOM  2854  N   ALA B 109    -16.029  85.227  30.333  1.00 22.44    B   N
ATOM  2855  CA  ALA B 109    -14.734  85.427  29.696  1.00 22.32    B   C
ATOM  2856  CB  ALA B 109    -14.179  86.795  30.062  1.00 19.60    B   C
ATOM  2857  C   ALA B 109    -13.768  84.334  30.133  1.00 21.09    B   C
ATOM  2858  O   ALA B 109    -13.580  84.107  31.326  1.00 21.33    B   O
ATOM  2859  N   PRO B 110    -13.152  83.635  29.168  1.00 21.10    B   N
ATOM  2860  CD  PRO B 110    -13.315  83.775  27.711  1.00 21.88    B   C
ATOM  2861  CA  PRO B 110    -12.201  82.562  29.485  1.00 21.55    B   C
ATOM  2862  CB  PRO B 110    -11.843  81.988  28.111  1.00 20.46    B   C
ATOM  2863  CG  PRO B 110    -13.002  82.387  27.233  1.00 23.31    B   C
ATOM  2864  C   PRO B 110    -10.974  83.142  30.190  1.00 21.39    B   C
ATOM  2865  O   PRO B 110    -10.243  83.950  29.615  1.00 20.23    B   O
ATOM  2866  N   ILE B 111    -10.757  82.731  31.433  1.00 20.74    B   N
ATOM  2867  CA  ILE B 111     -9.621  83.220  32.208  1.00 21.29    B   C
ATOM  2868  CB  ILE B 111    -10.085  83.770  33.575  1.00 18.70    B   C
ATOM  2869  CG2 ILE B 111     -8.883  84.214  34.398  1.00 19.35    B   C
ATOM  2870  CG1 ILE B 111    -11.054  84.937  33.365  1.00 17.87    B   C
ATOM  2871  CD1 ILE B 111    -11.768  85.374  34.632  1.00 13.74    B   C
ATOM  2872  C   ILE B 111     -8.618  82.096  32.439  1.00 20.50    B   C
ATOM  2873  O   ILE B 111     -8.983  81.017  32.900  1.00 21.37    B   O
ATOM  2874  N   LEU B 112     -7.358  82.354  32.107  1.00 19.57    B   N
ATOM  2875  CA  LEU B 112     -6.302  81.367  32.285  1.00 18.55    B   C
ATOM  2876  CB  LEU B 112     -5.538  81.154  30.975  1.00 17.95    B   C
ATOM  2877  CG  LEU B 112     -4.340  80.200  31.024  1.00 18.08    B   C
ATOM  2878  CD1 LEU B 112     -4.774  78.812  31.482  1.00 19.26    B   C
ATOM  2879  CD2 LEU B 112     -3.713  80.132  29.640  1.00 16.52    B   C
ATOM  2880  C   LEU B 112     -5.329  81.799  33.370  1.00 18.08    B   C
ATOM  2881  O   LEU B 112     -4.731  82.873  33.291  1.00 19.20    B   O
ATOM  2882  N   VAL B 113     -5.171  80.951  34.380  1.00 16.92    B   N
ATOM  2883  CA  VAL B 113     -4.269  81.231  35.487  1.00 16.68    B   C
ATOM  2884  CB  VAL B 113     -4.863  80.728  36.835  1.00 17.69    B   C
ATOM  2885  CG1 VAL B 113     -3.945  81.110  37.994  1.00 17.55    B   C
ATOM  2886  CG2 VAL B 113     -6.244  81.309  37.050  1.00 17.01    B   C
ATOM  2887  C   VAL B 113     -2.943  80.516  35.243  1.00 16.02    B   C
ATOM  2888  O   VAL B 113     -2.921  79.308  34.999  1.00 14.64    B   O
ATOM  2889  N   LEU B 114     -1.845  81.267  35.291  1.00 14.63    B   N
ATOM  2890  CA  LEU B 114     -0.520  80.692  35.104  1.00 13.92    B   C
ATOM  2891  CB  LEU B 114      0.247  81.395  33.979  1.00 11.65    B   C
ATOM  2892  CG  LEU B 114     -0.330  81.466  32.566  1.00 17.67    B   C
ATOM  2893  CD1 LEU B 114      0.736  82.064  31.644  1.00 16.72    B   C
ATOM  2894  CD2 LEU B 114     -0.738  80.081  32.077  1.00 17.71    B   C
ATOM  2895  C   LEU B 114      0.256  80.881  36.399  1.00 14.25    B   C
ATOM  2896  O   LEU B 114      0.210  81.947  37.005  1.00 11.47    B   O
ATOM  2897  N   GLY B 115      0.984  79.855  36.813  1.00 14.70    B   N
ATOM  2898  CA  GLY B 115      1.757  79.971  38.037  1.00 15.73    B   C
ATOM  2899  C   GLY B 115      2.608  78.746  38.289  1.00 14.74    B   C
ATOM  2900  O   GLY B 115      2.693  77.855  37.451  1.00 13.78    B   O
ATOM  2901  N   THR B 116      3.252  78.706  39.447  1.00 16.02    B   N
ATOM  2902  CA  THR B 116      4.087  77.568  39.798  1.00 15.11    B   C
ATOM  2903  CB  THR B 116      4.916  77.860  41.045  1.00 14.07    B   C
ATOM  2904  OG1 THR B 116      4.040  78.104  42.155  1.00 12.96    B   O
ATOM  2905  CG2 THR B 116      5.800  79.074  40.814  1.00 13.81    B   C
ATOM  2906  C   THR B 116      3.182  76.375  40.083  1.00 15.15    B   C
ATOM  2907  O   THR B 116      1.974  76.528  40.260  1.00 15.43    B   O
ATOM  2908  N   LYS B 117      3.768  75.189  40.124  1.00 14.92    B   N
ATOM  2909  CA  LYS B 117      2.998  73.991  40.401  1.00 16.68    B   C
ATOM  2910  CB  LYS B 117      3.926  72.776  40.462  1.00 18.20    B   C
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Figure 7ZZ

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ATOM  2911 CG  LYS B 117     3.170  71.459  40.516  1.00 28.15    B   C
ATOM  2912 CD  LYS B 117     2.286  71.334  39.280  1.00 34.68    B   C
ATOM  2913 CE  LYS B 117     1.422  70.089  39.310  1.00 37.95    B   C
ATOM  2914 NZ  LYS B 117     0.628  69.995  38.057  1.00 40.68    B   N
ATOM  2915 C   LYS B 117     2.231  74.125  41.725  1.00 15.54    B   C
ATOM  2916 O   LYS B 117     1.055  73.772  41.811  1.00 13.25    B   O
ATOM  2917 N   ALA B 118     2.896  74.648  42.753  1.00 13.55    B   N
ATOM  2918 CA  ALA B 118     2.263  74.797  44.062  1.00 13.07    B   C
ATOM  2919 CB  ALA B 118     3.294  75.271  45.092  1.00 13.77    B   C
ATOM  2920 C   ALA B 118     1.084  75.755  44.020  1.00 13.96    B   C
ATOM  2921 O   ALA B 118     0.022  75.478  44.584  1.00 12.32    B   O
ATOM  2922 N   THR B 119     1.270  76.887  43.347  1.00 12.40    B   N
ATOM  2923 CA  THR B 119     0.204  77.874  43.248  1.00 14.50    B   C
ATOM  2924 CB  THR B 119     0.698  79.159  42.534  1.00 11.89    B   C
ATOM  2925 OG1 THR B 119     1.739  79.763  43.311  1.00 13.56    B   O
ATOM  2926 CG2 THR B 119    -0.443  80.158  42.373  1.00 12.19    B   C
ATOM  2927 C   THR B 119    -1.005  77.312  42.504  1.00 12.61    B   C
ATOM  2928 O   THR B 119    -2.140  77.473  42.942  1.00 15.20    B   O
ATOM  2929 N   ILE B 120    -0.759  76.641  41.385  1.00 13.07    B   N
ATOM  2930 CA  ILE B 120    -1.847  76.080  40.594  1.00 17.11    B   C
ATOM  2931 CB  ILE B 120    -1.333  75.521  39.242  1.00 15.75    B   C
ATOM  2932 CG2 ILE B 120    -2.499  74.993  38.418  1.00 19.67    B   C
ATOM  2933 CG1 ILE B 120    -0.600  76.620  38.461  1.00 15.38    B   C
ATOM  2934 CD1 ILE B 120    -1.456  77.829  38.120  1.00 19.05    B   C
ATOM  2935 C   ILE B 120    -2.605  74.971  41.331  1.00 17.21    B   C
ATOM  2936 O   ILE B 120    -3.832  74.938  41.309  1.00 18.55    B   O
ATOM  2937 N   GLN B 121    -1.887  74.064  41.984  1.00 17.85    B   N
ATOM  2938 CA  GLN B 121    -2.554  72.983  42.700  1.00 21.02    B   C
ATOM  2939 CB  GLN B 121    -1.539  71.946  43.177  1.00 23.26    B   C
ATOM  2940 CG  GLN B 121    -0.796  71.267  42.053  1.00 31.27    B   C
ATOM  2941 CD  GLN B 121    -0.046  70.038  42.509  1.00 34.42    B   C
ATOM  2942 OE1 GLN B 121     0.702  70.078  43.488  1.00 38.77    B   O
ATOM  2943 NE2 GLN B 121    -0.237  68.933  41.797  1.00 36.80    B   N
ATOM  2944 C   GLN B 121    -3.375  73.477  43.894  1.00 21.84    B   C
ATOM  2945 O   GLN B 121    -4.297  72.795  44.345  1.00 23.51    B   O
ATOM  2946 N   SER B 122    -3.056  74.661  44.404  1.00 20.44    B   N
ATOM  2947 CA  SER B 122    -3.791  75.193  45.549  1.00 20.89    B   C
ATOM  2948 CB  SER B 122    -3.024  76.348  46.208  1.00 20.03    B   C
ATOM  2949 OG  SER B 122    -3.115  77.537  45.438  1.00 19.77    B   O
ATOM  2950 C   SER B 122    -5.178  75.687  45.152  1.00 19.13    B   C
ATOM  2951 O   SER B 122    -6.057  75.812  46.000  1.00 18.67    B   O
ATOM  2952 N   ASN B 123    -5.362  75.960  43.864  1.00 20.34    B   N
ATOM  2953 CA  ASN B 123    -6.626  76.476  43.345  1.00 21.65    B   C
ATOM  2954 CB  ASN B 123    -7.756  75.464  43.543  1.00 24.19    B   C
ATOM  2955 CG  ASN B 123    -7.662  74.302  42.583  1.00 28.22    B   C
ATOM  2956 OD1 ASN B 123    -7.618  74.492  41.368  1.00 28.03    B   O
ATOM  2957 ND2 ASN B 123    -7.632  73.087  43.121  1.00 31.95    B   N
ATOM  2958 C   ASN B 123    -6.990  77.787  44.025  1.00 20.93    B   C
ATOM  2959 O   ASN B 123    -8.162  78.160  44.098  1.00 20.81    B   O
ATOM  2960 N   ALA B 124    -5.977  78.488  44.520  1.00 18.37    B   N
ATOM  2961 CA  ALA B 124    -6.205  79.759  45.187  1.00 19.77    B   C
ATOM  2962 CB  ALA B 124    -4.872  80.387  45.588  1.00 18.94    B   C
ATOM  2963 C   ALA B 124    -6.993  80.715  44.285  1.00 18.40    B   C
ATOM  2964 O   ALA B 124    -8.032  81.239  44.685  1.00 20.72    B   O
ATOM  2965 N   TYR B 125    -6.506  80.936  43.069  1.00 19.24    B   N
ATOM  2966 CA  TYR B 125    -7.184  81.841  42.142  1.00 19.32    B   C
ATOM  2967 CB  TYR B 125    -6.331  82.091  40.892  1.00 19.37    B   C
ATOM  2968 CG  TYR B 125    -5.129  82.989  41.102  1.00 19.31    B   C
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Figure 7AAA

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ATOM  2969 CD1 TYR B 125     -3.887  82.457  41.439  1.00 17.61      B   C
ATOM  2970 CE1 TYR B 125     -2.768  83.280  41.591  1.00 18.62      B   C
ATOM  2971 CD2 TYR B 125     -5.228  84.371  40.929  1.00 17.15      B   C
ATOM  2972 CE2 TYR B 125     -4.123  85.197  41.078  1.00 16.64      B   C
ATOM  2973 CZ  TYR B 125     -2.895  84.646  41.405  1.00 17.43      B   C
ATOM  2974 OH  TYR B 125     -1.792  85.454  41.520  1.00 17.10      B   O
ATOM  2975 C   TYR B 125     -8.553  81.340  41.696  1.00 19.25      B   C
ATOM  2976 O   TYR B 125     -9.528  82.096  41.688  1.00 18.74      B   O
ATOM  2977 N   ASP B 126     -8.617  80.071  41.310  1.00 18.47      B   N
ATOM  2978 CA  ASP B 126     -9.862  79.473  40.841  1.00 19.68      B   C
ATOM  2979 CB  ASP B 126     -9.660  77.986  40.552  1.00 19.72      B   C
ATOM  2980 CG  ASP B 126     -8.455  77.720  39.671  1.00 23.51      B   C
ATOM  2981 OD1 ASP B 126     -7.341  78.138  40.042  1.00 24.96      B   O
ATOM  2982 OD2 ASP B 126     -8.621  77.085  38.609  1.00 22.93      B   O
ATOM  2983 C   ASP B 126    -10.972  79.635  41.868  1.00 21.84      B   C
ATOM  2984 O   ASP B 126    -12.076  80.077  41.541  1.00 18.17      B   O
ATOM  2985 N   ASN B 127    -10.676  79.273  43.113  1.00 21.58      B   N
ATOM  2986 CA  ASN B 127    -11.659  79.376  44.181  1.00 22.68      B   C
ATOM  2987 CB  ASN B 127    -11.081  78.839  45.495  1.00 22.98      B   C
ATOM  2988 CG  ASN B 127    -10.656  77.385  45.393  1.00 26.68      B   C
ATOM  2989 OD1 ASN B 127    -11.290  76.591  44.701  1.00 26.92      B   O
ATOM  2990 ND2 ASN B 127     -9.582  77.029  46.092  1.00 29.75      B   N
ATOM  2991 C   ASN B 127    -12.105  80.821  44.362  1.00 22.20      B   C
ATOM  2992 O   ASN B 127    -13.300  81.104  44.443  1.00 22.96      B   O
ATOM  2993 N   ALA B 128    -11.145  81.736  44.422  1.00 21.77      B   N
ATOM  2994 CA  ALA B 128    -11.465  83.149  44.587  1.00 22.81      B   C
ATOM  2995 CB  ALA B 128    -10.184  83.970  44.693  1.00 24.04      B   C
ATOM  2996 C   ALA B 128    -12.315  83.643  43.422  1.00 24.10      B   C
ATOM  2997 O   ALA B 128    -13.302  84.354  43.624  1.00 27.04      B   O
ATOM  2998 N   LEU B 129    -11.935  83.262  42.205  1.00 24.54      B   N
ATOM  2999 CA  LEU B 129    -12.672  83.664  41.012  1.00 24.58      B   C
ATOM  3000 CB  LEU B 129    -11.926  83.225  39.753  1.00 22.03      B   C
ATOM  3001 CG  LEU B 129    -10.633  83.975  39.418  1.00 24.03      B   C
ATOM  3002 CD1 LEU B 129     -9.865  83.210  38.366  1.00 22.36      B   C
ATOM  3003 CD2 LEU B 129    -10.956  85.382  38.932  1.00 22.58      B   C
ATOM  3004 C   LEU B 129    -14.078  83.070  41.005  1.00 26.08      B   C
ATOM  3005 O   LEU B 129    -15.046  83.751  40.669  1.00 26.16      B   O
ATOM  3006 N   LYS B 130    -14.185  81.795  41.365  1.00 26.80      B   N
ATOM  3007 CA  LYS B 130    -15.482  81.130  41.404  1.00 29.37      B   C
ATOM  3008 CB  LYS B 130    -15.326  79.694  41.904  1.00 32.59      B   C
ATOM  3009 CG  LYS B 130    -16.638  78.939  42.019  1.00 37.42      B   C
ATOM  3010 CD  LYS B 130    -17.337  78.877  40.675  1.00 43.42      B   C
ATOM  3011 CE  LYS B 130    -18.708  78.237  40.775  1.00 45.02      B   C
ATOM  3012 NZ  LYS B 130    -19.379  78.220  39.444  1.00 49.29      B   N
ATOM  3013 C   LYS B 130    -16.400  81.897  42.347  1.00 29.56      B   C
ATOM  3014 O   LYS B 130    -17.538  82.218  42.010  1.00 28.29      B   O
ATOM  3015 N   GLN B 131    -15.876  82.185  43.532  1.00 29.31      B   N
ATOM  3016 CA  GLN B 131    -16.599  82.911  44.559  1.00 31.88      B   C
ATOM  3017 CB  GLN B 131    -15.667  83.162  45.747  1.00 35.97      B   C
ATOM  3018 CG  GLN B 131    -16.286  83.913  46.918  1.00 45.23      B   C
ATOM  3019 CD  GLN B 131    -17.385  83.128  47.610  1.00 50.61      B   C
ATOM  3020 OE1 GLN B 131    -17.211  81.951  47.942  1.00 53.57      B   O
ATOM  3021 NE2 GLN B 131    -18.524  83.781  47.843  1.00 52.00      B   N
ATOM  3022 C   GLN B 131    -17.137  84.239  44.035  1.00 31.40      B   C
ATOM  3023 O   GLN B 131    -18.222  84.675  44.427  1.00 29.81      B   O
ATOM  3024 N   GLN B 132    -16.382  84.878  43.145  1.00 29.49      B   N
ATOM  3025 CA  GLN B 132    -16.788  86.166  42.597  1.00 29.13      B   C
ATOM  3026 CB  GLN B 132    -15.558  87.020  42.290  1.00 30.78      B   C
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Figure 7BBB

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ATOM  3027 CG  GLN B 132   -14.776  87.410  43.535  1.00 32.44    B   C
ATOM  3028 CD  GLN B 132   -15.644  88.114  44.565  1.00 35.76    B   C
ATOM  3029 OE1 GLN B 132   -16.234  89.158  44.286  1.00 35.79    B   O
ATOM  3030 NE2 GLN B 132   -15.725  87.542  45.763  1.00 34.46    B   N
ATOM  3031 C   GLN B 132   -17.682  86.079  41.368  1.00 29.17    B   C
ATOM  3032 O   GLN B 132   -17.994  87.096  40.747  1.00 28.85    B   O
ATOM  3033 N   GLY B 133   -18.075  84.864  41.004  1.00 28.71    B   N
ATOM  3034 CA  GLY B 133   -18.974  84.700  39.879  1.00 28.15    B   C
ATOM  3035 C   GLY B 133   -18.442  84.343  38.509  1.00 27.61    B   C
ATOM  3036 O   GLY B 133   -19.224  84.310  37.561  1.00 26.00    B   O
ATOM  3037 N   TYR B 134   -17.146  84.078  38.371  1.00 26.83    B   N
ATOM  3038 CA  TYR B 134   -16.627  83.721  37.056  1.00 26.16    B   C
ATOM  3039 CB  TYR B 134   -15.135  84.049  36.961  1.00 24.55    B   C
ATOM  3040 CG  TYR B 134   -14.921  85.545  36.938  1.00 22.77    B   C
ATOM  3041 CD1 TYR B 134   -14.840  86.277  38.123  1.00 22.62    B   C
ATOM  3042 CE1 TYR B 134   -14.760  87.670  38.109  1.00 23.49    B   C
ATOM  3043 CD2 TYR B 134   -14.911  86.246  35.730  1.00 24.51    B   C
ATOM  3044 CE2 TYR B 134   -14.834  87.641  35.702  1.00 25.08    B   C
ATOM  3045 CZ  TYR B 134   -14.759  88.346  36.896  1.00 23.66    B   C
ATOM  3046 OH  TYR B 134   -14.689  89.721  36.886  1.00 24.39    B   O
ATOM  3047 C   TYR B 134   -16.927  82.264  36.729  1.00 26.95    B   C
ATOM  3048 O   TYR B 134   -16.774  81.379  37.571  1.00 26.50    B   O
ATOM  3049 N   LEU B 135   -17.362  82.031  35.494  1.00 25.91    B   N
ATOM  3050 CA  LEU B 135   -17.777  80.704  35.049  1.00 28.31    B   C
ATOM  3051 CB  LEU B 135   -19.155  80.822  34.388  1.00 28.49    B   C
ATOM  3052 CG  LEU B 135   -20.131  81.733  35.139  1.00 28.21    B   C
ATOM  3053 CD1 LEU B 135   -21.343  82.031  34.272  1.00 28.13    B   C
ATOM  3054 CD2 LEU B 135   -20.527  81.077  36.455  1.00 29.07    B   C
ATOM  3055 C   LEU B 135   -16.847  79.940  34.113  1.00 27.36    B   C
ATOM  3056 O   LEU B 135   -17.066  78.758  33.855  1.00 27.87    B   O
ATOM  3057 N   ASN B 136   -15.819  80.602  33.596  1.00 28.12    B   N
ATOM  3058 CA  ASN B 136   -14.892  79.944  32.681  1.00 25.99    B   C
ATOM  3059 CB  ASN B 136   -15.053  80.520  31.276  1.00 27.18    B   C
ATOM  3060 CG  ASN B 136   -14.416  79.652  30.214  1.00 27.92    B   C
ATOM  3061 OD1 ASN B 136   -13.572  78.807  30.509  1.00 28.48    B   O
ATOM  3062 ND2 ASN B 136   -14.809  79.866  28.962  1.00 30.11    B   N
ATOM  3063 C   ASN B 136   -13.460  80.159  33.172  1.00 26.03    B   C
ATOM  3064 O   ASN B 136   -12.749  81.040  32.688  1.00 24.61    B   O
ATOM  3065 N   ILE B 137   -13.046  79.342  34.133  1.00 24.40    B   N
ATOM  3066 CA  ILE B 137   -11.715  79.451  34.716  1.00 24.19    B   C
ATOM  3067 CB  ILE B 137   -11.816  79.575  36.254  1.00 25.00    B   C
ATOM  3068 CG2 ILE B 137   -10.430  79.802  36.857  1.00 26.36    B   C
ATOM  3069 CG1 ILE B 137   -12.752  80.735  36.616  1.00 25.12    B   C
ATOM  3070 CD1 ILE B 137   -13.231  80.738  38.056  1.00 25.56    B   C
ATOM  3071 C   ILE B 137   -10.809  78.268  34.378  1.00 24.30    B   C
ATOM  3072 O   ILE B 137   -11.180  77.114  34.574  1.00 24.24    B   O
ATOM  3073 N   SER B 138   -9.620  78.570  33.865  1.00 22.99    B   N
ATOM  3074 CA  SER B 138   -8.640  77.545  33.520  1.00 23.07    B   C
ATOM  3075 CB  SER B 138   -8.357  77.547  32.016  1.00 21.90    B   C
ATOM  3076 OG  SER B 138   -9.532  77.297  31.271  1.00 28.80    B   O
ATOM  3077 C   SER B 138   -7.345  77.845  34.267  1.00 21.12    B   C
ATOM  3078 O   SER B 138   -7.104  78.986  34.675  1.00 18.88    B   O
ATOM  3079 N   HIS B 139   -6.521  76.820  34.463  1.00 20.44    B   N
ATOM  3080 CA  HIS B 139   -5.242  77.010  35.134  1.00 20.66    B   C
ATOM  3081 CB  HIS B 139   -5.343  76.712  36.639  1.00 20.23    B   C
ATOM  3082 CG  HIS B 139   -5.802  75.322  36.964  1.00 21.50    B   C
ATOM  3083 CD2 HIS B 139   -5.241  74.114  36.716  1.00 22.63    B   C
ATOM  3084 ND1 HIS B 139   -6.984  75.067  37.626  1.00 20.86    B   N
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Figure 7CCC

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ATOM  3085 CE1 HIS B 139     -7.132  73.761  37.770  1.00 23.65    B   C
ATOM  3086 NE2 HIS B 139     -6.089  73.161  37.226  1.00 23.23    B   N
ATOM  3087 C   HIS B 139     -4.172  76.148  34.488  1.00 21.34    B   C
ATOM  3088 O   HIS B 139     -4.468  75.120  33.874  1.00 21.81    B   O
ATOM  3089 N   LEU B 140     -2.922  76.578  34.614  1.00 21.36    B   N
ATOM  3090 CA  LEU B 140     -1.815  75.846  34.023  1.00 20.20    B   C
ATOM  3091 CB  LEU B 140     -1.644  76.244  32.558  1.00 21.19    B   C
ATOM  3092 CG  LEU B 140     -0.502  75.564  31.800  1.00 21.50    B   C
ATOM  3093 CD1 LEU B 140     -0.790  74.074  31.688  1.00 21.95    B   C
ATOM  3094 CD2 LEU B 140     -0.357  76.190  30.410  1.00 21.96    B   C
ATOM  3095 C   LEU B 140     -0.511  76.104  34.758  1.00 19.11    B   C
ATOM  3096 O   LEU B 140     -0.098  77.248  34.928  1.00 16.59    B   O
ATOM  3097 N   ALA B 141      0.135  75.027  35.186  1.00 19.36    B   N
ATOM  3098 CA  ALA B 141      1.405  75.133  35.887  1.00 19.87    B   C
ATOM  3099 CB  ALA B 141      1.603  73.918  36.791  1.00 21.48    B   C
ATOM  3100 C   ALA B 141      2.531  75.215  34.856  1.00 16.62    B   C
ATOM  3101 O   ALA B 141      2.912  74.214  34.261  1.00 20.61    B   O
ATOM  3102 N   THR B 142      3.049  76.415  34.630  1.00 15.84    B   N
ATOM  3103 CA  THR B 142      4.132  76.600  33.676  1.00 14.20    B   C
ATOM  3104 CB  THR B 142      3.948  77.913  32.889  1.00 13.97    B   C
ATOM  3105 OG1 THR B 142      3.814  79.003  33.806  1.00 14.25    B   O
ATOM  3106 CG2 THR B 142      2.691  77.840  32.023  1.00 13.62    B   C
ATOM  3107 C   THR B 142      5.410  76.652  34.505  1.00 14.37    B   C
ATOM  3108 O   THR B 142      6.114  77.653  34.529  1.00 13.97    B   O
ATOM  3109 N   SER B 143      5.698  75.544  35.176  1.00 15.59    B   N
ATOM  3110 CA  SER B 143      6.844  75.444  36.067  1.00 16.89    B   C
ATOM  3111 CB  SER B 143      6.971  74.013  36.591  1.00 19.31    B   C
ATOM  3112 OG  SER B 143      8.003  73.931  37.564  1.00 27.09    B   O
ATOM  3113 C   SER B 143      8.193  75.902  35.537  1.00 16.21    B   C
ATOM  3114 O   SER B 143      8.892  76.666  36.205  1.00 16.07    B   O
ATOM  3115 N   LEU B 144      8.557  75.446  34.345  1.00 15.08    B   N
ATOM  3116 CA  LEU B 144      9.850  75.783  33.759  1.00 15.48    B   C
ATOM  3117 CB  LEU B 144     10.094  74.929  32.520  1.00 15.32    B   C
ATOM  3118 CG  LEU B 144     10.215  73.436  32.827  1.00 16.70    B   C
ATOM  3119 CD1 LEU B 144     10.267  72.642  31.536  1.00 19.80    B   C
ATOM  3120 CD2 LEU B 144     11.468  73.190  33.654  1.00 19.07    B   C
ATOM  3121 C   LEU B 144     10.037  77.251  33.421  1.00 14.68    B   C
ATOM  3122 O   LEU B 144     11.145  77.678  33.098  1.00 14.35    B   O
ATOM  3123 N   PHE B 145      8.962  78.028  33.484  1.00 14.12    B   N
ATOM  3124 CA  PHE B 145      9.088  79.447  33.199  1.00 15.35    B   C
ATOM  3125 CB  PHE B 145      7.719  80.148  33.232  1.00 13.56    B   C
ATOM  3126 CG  PHE B 145      6.911  79.992  31.964  1.00 14.58    B   C
ATOM  3127 CD1 PHE B 145      5.657  80.594  31.852  1.00 13.83    B   C
ATOM  3128 CD2 PHE B 145      7.393  79.252  30.888  1.00 16.08    B   C
ATOM  3129 CE1 PHE B 145      4.899  80.461  30.688  1.00 14.15    B   C
ATOM  3130 CE2 PHE B 145      6.646  79.111  29.720  1.00 15.95    B   C
ATOM  3131 CZ  PHE B 145      5.395  79.717  29.620  1.00 14.39    B   C
ATOM  3132 C   PHE B 145     10.011  80.084  34.233  1.00 14.15    B   C
ATOM  3133 O   PHE B 145     10.821  80.942  33.896  1.00 13.84    B   O
ATOM  3134 N   VAL B 146      9.901  79.648  35.488  1.00 14.43    B   N
ATOM  3135 CA  VAL B 146     10.721  80.215  36.558  1.00 15.36    B   C
ATOM  3136 CB  VAL B 146     10.353  79.617  37.949  1.00 17.29    B   C
ATOM  3137 CG1 VAL B 146     11.367  80.065  38.995  1.00 16.50    B   C
ATOM  3138 CG2 VAL B 146      8.959  80.079  38.369  1.00 14.60    B   C
ATOM  3139 C   VAL B 146     12.229  80.086  36.329  1.00 14.39    B   C
ATOM  3140 O   VAL B 146     12.935  81.092  36.326  1.00 14.20    B   O
ATOM  3141 N   PRO B 147     12.747  78.856  36.144  1.00 14.14    B   N
ATOM  3142 CD  PRO B 147     12.141  77.519  36.269  1.00 13.43    B   C
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Figure 7DDD

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ATOM  3143  CA  PRO B 147     14.195  78.754  35.921  1.00 14.59      B   C
ATOM  3144  CB  PRO B 147     14.457  77.242  35.995  1.00 13.53      B   C
ATOM  3145  CG  PRO B 147     13.151  76.642  35.573  1.00 14.07      B   C
ATOM  3146  C   PRO B 147     14.653  79.377  34.597  1.00 13.40      B   C
ATOM  3147  O   PRO B 147     15.775  79.877  34.500  1.00 13.19      B   O
ATOM  3148  N   LEU B 148     13.796  79.355  33.577  1.00 11.38      B   N
ATOM  3149  CA  LEU B 148     14.179  79.960  32.303  1.00 12.63      B   C
ATOM  3150  CB  LEU B 148     13.100  79.751  31.232  1.00 14.70      B   C
ATOM  3151  CG  LEU B 148     13.404  78.655  30.202  1.00 12.09      B   C
ATOM  3152  CD1 LEU B 148     13.446  77.315  30.903  1.00 14.46      B   C
ATOM  3153  CD2 LEU B 148     12.341  78.649  29.106  1.00 18.20      B   C
ATOM  3154  C   LEU B 148     14.395  81.448  32.508  1.00 12.91      B   C
ATOM  3155  O   LEU B 148     15.372  82.018  32.031  1.00 12.96      B   O
ATOM  3156  N   ILE B 149     13.471  82.070  33.231  1.00 13.00      B   N
ATOM  3157  CA  ILE B 149     13.545  83.500  33.499  1.00 12.87      B   C
ATOM  3158  CB  ILE B 149     12.211  83.989  34.130  1.00 13.86      B   C
ATOM  3159  CG2 ILE B 149     12.352  85.419  34.647  1.00 12.28      B   C
ATOM  3160  CG1 ILE B 149     11.099  83.891  33.071  1.00 14.05      B   C
ATOM  3161  CD1 ILE B 149      9.694  84.067  33.608  1.00 15.21      B   C
ATOM  3162  C   ILE B 149     14.742  83.842  34.386  1.00 12.66      B   C
ATOM  3163  O   ILE B 149     15.403  84.852  34.172  1.00 11.51      B   O
ATOM  3164  N   GLU B 150     15.041  82.995  35.366  1.00 12.92      B   N
ATOM  3165  CA  GLU B 150     16.180  83.266  36.235  1.00 13.66      B   C
ATOM  3166  CB  GLU B 150     16.182  82.313  37.441  1.00 18.92      B   C
ATOM  3167  CG  GLU B 150     14.884  82.371  38.242  1.00 23.46      B   C
ATOM  3168  CD  GLU B 150     15.024  81.875  39.673  1.00 28.25      B   C
ATOM  3169  OE1 GLU B 150     15.728  80.863  39.887  1.00 30.76      B   O
ATOM  3170  OE2 GLU B 150     14.414  82.491  40.581  1.00 24.21      B   O
ATOM  3171  C   GLU B 150     17.491  83.163  35.462  1.00 13.99      B   C
ATOM  3172  O   GLU B 150     18.484  83.776  35.844  1.00 14.58      B   O
ATOM  3173  N   GLU B 151     17.500  82.403  34.370  1.00 13.36      B   N
ATOM  3174  CA  GLU B 151     18.712  82.277  33.571  1.00 16.12      B   C
ATOM  3175  CB  GLU B 151     18.863  80.861  33.006  1.00 18.99      B   C
ATOM  3176  CG  GLU B 151     20.276  80.598  32.500  1.00 25.66      B   C
ATOM  3177  CD  GLU B 151     20.615  79.128  32.403  1.00 27.80      B   C
ATOM  3178  OE1 GLU B 151     20.307  78.389  33.362  1.00 33.36      B   O
ATOM  3179  OE2 GLU B 151     21.204  78.716  31.378  1.00 24.62      B   O
ATOM  3180  C   GLU B 151     18.695  83.293  32.436  1.00 15.49      B   C
ATOM  3181  O   GLU B 151     19.515  83.243  31.522  1.00 16.76      B   O
ATOM  3182  N   SER B 152     17.746  84.218  32.514  1.00 15.83      B   N
ATOM  3183  CA  SER B 152     17.591  85.277  31.523  1.00 16.90      B   C
ATOM  3184  CB  SER B 152     18.843  86.159  31.486  1.00 16.89      B   C
ATOM  3185  OG  SER B 152     18.547  87.404  30.872  1.00 19.93      B   O
ATOM  3186  C   SER B 152     17.274  84.786  30.108  1.00 15.72      B   C
ATOM  3187  O   SER B 152     17.776  85.339  29.128  1.00 16.57      B   O
ATOM  3188  N   ILE B 153     16.452  83.746  30.003  1.00 16.59      B   N
ATOM  3189  CA  ILE B 153     16.048  83.223  28.701  1.00 16.23      B   C
ATOM  3190  CB  ILE B 153     15.840  81.688  28.747  1.00 17.80      B   C
ATOM  3191  CG2 ILE B 153     15.479  81.164  27.366  1.00 16.97      B   C
ATOM  3192  CG1 ILE B 153     17.118  81.008  29.247  1.00 18.17      B   C
ATOM  3193  CD1 ILE B 153     18.328  81.264  28.379  1.00 20.45      B   C
ATOM  3194  C   ILE B 153     14.716  83.924  28.465  1.00 17.00      B   C
ATOM  3195  O   ILE B 153     13.647  83.337  28.649  1.00 16.86      B   O
ATOM  3196  N   LEU B 154     14.802  85.192  28.074  1.00 16.13      B   N
ATOM  3197  CA  LEU B 154     13.629  86.036  27.861  1.00 17.93      B   C
ATOM  3198  CB  LEU B 154     13.891  87.412  28.475  1.00 15.30      B   C
ATOM  3199  CG  LEU B 154     14.390  87.335  29.923  1.00 14.99      B   C
ATOM  3200  CD1 LEU B 154     14.685  88.728  30.459  1.00 17.09      B   C
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Figure 7EEE

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ATOM  3201 CD2 LEU B 154    13.348  86.640  30.776  1.00 18.19    B   C
ATOM  3202 C   LEU B 154    13.188  86.204  26.413  1.00 19.02    B   C
ATOM  3203 O   LEU B 154    12.258  86.956  26.125  1.00 18.98    B   O
ATOM  3204 N   GLU B 155    13.857  85.506  25.506  1.00 19.46    B   N
ATOM  3205 CA  GLU B 155    13.520  85.579  24.093  1.00 20.61    B   C
ATOM  3206 CB  GLU B 155    14.055  86.877  23.481  1.00 23.20    B   C
ATOM  3207 CG  GLU B 155    15.563  86.894  23.285  1.00 31.50    B   C
ATOM  3208 CD  GLU B 155    16.077  88.235  22.778  1.00 39.23    B   C
ATOM  3209 OE1 GLU B 155    15.483  88.786  21.824  1.00 42.91    B   O
ATOM  3210 OE2 GLU B 155    17.084  88.734  23.328  1.00 43.36    B   O
ATOM  3211 C   GLU B 155    14.177  84.391  23.421  1.00 19.99    B   C
ATOM  3212 O   GLU B 155    14.864  83.610  24.077  1.00 21.64    B   O
ATOM  3213 N   GLY B 156    13.946  84.242  22.121  1.00 20.12    B   N
ATOM  3214 CA  GLY B 156    14.563  83.152  21.396  1.00 19.17    B   C
ATOM  3215 C   GLY B 156    13.844  81.820  21.366  1.00 20.79    B   C
ATOM  3216 O   GLY B 156    12.804  81.618  21.995  1.00 18.13    B   O
ATOM  3217 N   GLU B 157    14.451  80.898  20.626  1.00 22.19    B   N
ATOM  3218 CA  GLU B 157    13.946  79.548  20.415  1.00 21.56    B   C
ATOM  3219 CB  GLU B 157    14.952  78.782  19.553  1.00 25.02    B   C
ATOM  3220 CG  GLU B 157    14.524  77.377  19.184  1.00 35.87    B   C
ATOM  3221 CD  GLU B 157    15.499  76.703  18.231  1.00 41.09    B   C
ATOM  3222 OE1 GLU B 157    16.701  76.596  18.573  1.00 42.82    B   O
ATOM  3223 OE2 GLU B 157    15.058  76.275  17.141  1.00 42.70    B   O
ATOM  3224 C   GLU B 157    13.613  78.732  21.666  1.00 20.08    B   C
ATOM  3225 O   GLU B 157    12.588  78.044  21.702  1.00 18.27    B   O
ATOM  3226 N   LEU B 158    14.471  78.796  22.683  1.00 17.09    B   N
ATOM  3227 CA  LEU B 158    14.238  78.033  23.904  1.00 15.87    B   C
ATOM  3228 CB  LEU B 158    15.447  78.132  24.842  1.00 18.05    B   C
ATOM  3229 CG  LEU B 158    15.334  77.315  26.136  1.00 17.16    B   C
ATOM  3230 CD1 LEU B 158    14.977  75.872  25.807  1.00 15.66    B   C
ATOM  3231 CD2 LEU B 158    16.651  77.382  26.905  1.00 17.03    B   C
ATOM  3232 C   LEU B 158    12.973  78.488  24.630  1.00 16.52    B   C
ATOM  3233 O   LEU B 158    12.189  77.662  25.108  1.00 14.49    B   O
ATOM  3234 N   LEU B 159    12.775  79.799  24.727  1.00 14.92    B   N
ATOM  3235 CA  LEU B 159    11.580  80.306  25.383  1.00 14.51    B   C
ATOM  3236 CB  LEU B 159    11.660  81.823  25.578  1.00 15.13    B   C
ATOM  3237 CG  LEU B 159    10.374  82.456  26.133  1.00 16.38    B   C
ATOM  3238 CD1 LEU B 159     9.996  81.799  27.450  1.00 14.88    B   C
ATOM  3239 CD2 LEU B 159    10.574  83.955  26.326  1.00 15.09    B   C
ATOM  3240 C   LEU B 159    10.367  79.951  24.519  1.00 14.59    B   C
ATOM  3241 O   LEU B 159     9.350  79.492  25.028  1.00 13.56    B   O
ATOM  3242 N   GLU B 160    10.483  80.150  23.209  1.00 14.14    B   N
ATOM  3243 CA  GLU B 160     9.382  79.820  22.304  1.00 16.06    B   C
ATOM  3244 CB  GLU B 160     9.779  80.107  20.853  1.00 18.15    B   C
ATOM  3245 CG  GLU B 160     8.709  79.743  19.815  1.00 23.84    B   C
ATOM  3246 CD  GLU B 160     7.357  80.384  20.107  1.00 27.35    B   C
ATOM  3247 OE1 GLU B 160     7.330  81.496  20.683  1.00 24.13    B   O
ATOM  3248 OE2 GLU B 160     6.321  79.783  19.748  1.00 30.37    B   O
ATOM  3249 C   GLU B 160     8.987  78.348  22.438  1.00 15.10    B   C
ATOM  3250 O   GLU B 160     7.811  78.015  22.566  1.00 16.67    B   O
ATOM  3251 N   THR B 161     9.979  77.469  22.416  1.00 15.36    B   N
ATOM  3252 CA  THR B 161     9.720  76.037  22.518  1.00 16.10    B   C
ATOM  3253 CB  THR B 161    11.024  75.243  22.343  1.00 17.81    B   C
ATOM  3254 OG1 THR B 161    11.607  75.567  21.072  1.00 19.62    B   O
ATOM  3255 CG2 THR B 161    10.756  73.748  22.407  1.00 18.12    B   C
ATOM  3256 C   THR B 161     9.066  75.676  23.851  1.00 14.89    B   C
ATOM  3257 O   THR B 161     8.172  74.821  23.907  1.00 13.07    B   O
ATOM  3258 N   CYS B 162     9.500  76.342  24.918  1.00 12.65    B   N
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Figure 7FFF

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ATOM  3259 CA  CYS B 162     8.958  76.087  26.248  1.00 15.38    B   C
ATOM  3260 CB  CYS B 162     9.800  76.796  27.310  1.00 14.79    B   C
ATOM  3261 SG  CYS B 162     9.400  76.328  29.021  1.00 16.89    B   S
ATOM  3262 C   CYS B 162     7.505  76.557  26.341  1.00 15.60    B   C
ATOM  3263 O   CYS B 162     6.651  75.849  26.877  1.00 15.21    B   O
ATOM  3264 N   MET B 163     7.226  77.756  25.831  1.00 15.17    B   N
ATOM  3265 CA  MET B 163     5.863  78.271  25.860  1.00 15.78    B   C
ATOM  3266 CB  MET B 163     5.792  79.695  25.294  1.00 15.75    B   C
ATOM  3267 CG  MET B 163     6.424  80.767  26.162  1.00 16.77    B   C
ATOM  3268 SD  MET B 163     5.978  82.432  25.603  1.00 16.61    B   S
ATOM  3269 CE  MET B 163     6.937  82.509  24.114  1.00 14.38    B   C
ATOM  3270 C   MET B 163     4.962  77.360  25.033  1.00 14.99    B   C
ATOM  3271 O   MET B 163     3.819  77.093  25.410  1.00 15.77    B   O
ATOM  3272 N   HIS B 164     5.484  76.879  23.909  1.00 15.34    B   N
ATOM  3273 CA  HIS B 164     4.718  76.002  23.033  1.00 19.25    B   C
ATOM  3274 CB  HIS B 164     5.504  75.724  21.751  1.00 20.62    B   C
ATOM  3275 CG  HIS B 164     4.693  75.055  20.688  1.00 28.25    B   C
ATOM  3276 CD2 HIS B 164     4.779  73.817  20.146  1.00 28.01    B   C
ATOM  3277 ND1 HIS B 164     3.608  75.661  20.090  1.00 29.20    B   N
ATOM  3278 CE1 HIS B 164     3.060  74.824  19.227  1.00 29.23    B   C
ATOM  3279 NE2 HIS B 164     3.750  73.698  19.243  1.00 29.55    B   N
ATOM  3280 C   HIS B 164     4.412  74.690  23.760  1.00 19.47    B   C
ATOM  3281 O   HIS B 164     3.293  74.169  23.704  1.00 17.49    B   O
ATOM  3282 N   TYR B 165     5.419  74.169  24.449  1.00 17.68    B   N
ATOM  3283 CA  TYR B 165     5.277  72.937  25.210  1.00 16.69    B   C
ATOM  3284 CB  TYR B 165     6.578  72.655  25.969  1.00 15.68    B   C
ATOM  3285 CG  TYR B 165     6.457  71.544  26.976  1.00 17.57    B   C
ATOM  3286 CD1 TYR B 165     6.384  70.211  26.569  1.00 16.95    B   C
ATOM  3287 CE1 TYR B 165     6.216  69.191  27.498  1.00 20.45    B   C
ATOM  3288 CD2 TYR B 165     6.362  71.829  28.336  1.00 15.75    B   C
ATOM  3289 CE2 TYR B 165     6.193  70.818  29.273  1.00 17.81    B   C
ATOM  3290 CZ  TYR B 165     6.119  69.501  28.847  1.00 18.80    B   C
ATOM  3291 OH  TYR B 165     5.941  68.500  29.773  1.00 19.07    B   O
ATOM  3292 C   TYR B 165     4.101  73.027  26.193  1.00 16.83    B   C
ATOM  3293 O   TYR B 165     3.303  72.094  26.310  1.00 19.76    B   O
ATOM  3294 N   TYR B 166     3.999  74.151  26.895  1.00 16.40    B   N
ATOM  3295 CA  TYR B 166     2.931  74.369  27.864  1.00 16.70    B   C
ATOM  3296 CB  TYR B 166     3.362  75.435  28.888  1.00 13.68    B   C
ATOM  3297 CG  TYR B 166     4.354  74.961  29.930  1.00 15.63    B   C
ATOM  3298 CD1 TYR B 166     5.545  75.650  30.150  1.00 13.48    B   C
ATOM  3299 CE1 TYR B 166     6.458  75.218  31.113  1.00 17.41    B   C
ATOM  3300 CD2 TYR B 166     4.097  73.825  30.702  1.00 16.97    B   C
ATOM  3301 CE2 TYR B 166     5.001  73.387  31.668  1.00 14.41    B   C
ATOM  3302 CZ  TYR B 166     6.176  74.084  31.868  1.00 15.99    B   C
ATOM  3303 OH  TYR B 166     7.058  73.648  32.827  1.00 15.83    B   O
ATOM  3304 C   TYR B 166     1.576  74.793  27.278  1.00 17.53    B   C
ATOM  3305 O   TYR B 166     0.529  74.344  27.746  1.00 18.77    B   O
ATOM  3306 N   PHE B 167     1.599  75.651  26.260  1.00 18.80    B   N
ATOM  3307 CA  PHE B 167     0.367  76.198  25.668  1.00 19.74    B   C
ATOM  3308 CB  PHE B 167     0.660  77.589  25.115  1.00 18.42    B   C
ATOM  3309 CG  PHE B 167     1.092  78.573  26.163  1.00 17.20    B   C
ATOM  3310 CD1 PHE B 167     1.928  79.627  25.824  1.00 16.80    B   C
ATOM  3311 CD2 PHE B 167     0.635  78.472  27.482  1.00 16.87    B   C
ATOM  3312 CE1 PHE B 167     2.306  80.572  26.770  1.00 17.05    B   C
ATOM  3313 CE2 PHE B 167     1.010  79.419  28.439  1.00 17.71    B   C
ATOM  3314 CZ  PHE B 167     1.851  80.472  28.075  1.00 17.51    B   C
ATOM  3315 C   PHE B 167    -0.367  75.383  24.618  1.00 21.10    B   C
ATOM  3316 O   PHE B 167    -1.597  75.430  24.535  1.00 19.22    B   O
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Figure 7GGG

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ATOM  3317 N   THR B 168     0.403  74.657  23.812  1.00 23.27    B   N
ATOM  3318 CA  THR B 168    -0.165  73.805  22.765  1.00 26.77    B   C
ATOM  3319 CB  THR B 168     0.865  72.832  22.187  1.00 27.57    B   C
ATOM  3320 OG1 THR B 168     1.911  73.535  21.517  1.00 32.03    B   O
ATOM  3321 CG2 THR B 168     0.186  71.880  21.180  1.00 32.54    B   C
ATOM  3322 C   THR B 168    -1.363  72.944  23.205  1.00 26.77    B   C
ATOM  3323 O   THR B 168    -2.395  72.938  22.572  1.00 28.26    B   O
ATOM  3324 N   PRO B 169    -1.239  72.197  24.326  1.00 26.46    B   N
ATOM  3325 CD  PRO B 169    -0.050  72.083  25.152  1.00 26.67    B   C
ATOM  3326 CA  PRO B 169    -2.291  71.326  24.883  1.00 25.55    B   C
ATOM  3327 CB  PRO B 169    -1.610  70.668  26.066  1.00 26.50    B   C
ATOM  3328 CG  PRO B 169    -0.169  70.666  25.699  1.00 26.43    B   C
ATOM  3329 C   PRO B 169    -3.593  72.077  25.297  1.00 24.82    B   C
ATOM  3330 O   PRO B 169    -4.610  71.418  25.576  1.00 24.34    B   O
ATOM  3331 N   LEU B 170    -3.536  73.405  25.391  1.00 22.80    B   N
ATOM  3332 CA  LEU B 170    -4.729  74.167  25.761  1.00 25.50    B   C
ATOM  3333 CB  LEU B 170    -4.385  75.632  25.964  1.00 23.84    B   C
ATOM  3334 CG  LEU B 170    -3.514  75.982  27.186  1.00 25.53    B   C
ATOM  3335 CD1 LEU B 170    -3.138  77.463  27.146  1.00 26.01    B   C
ATOM  3336 CD2 LEU B 170    -4.242  75.652  28.503  1.00 26.09    B   C
ATOM  3337 C   LEU B 170    -5.772  74.057  24.644  1.00 25.77    B   C
ATOM  3338 O   LEU B 170    -5.436  74.103  23.453  1.00 26.97    B   O
ATOM  3339 N   GLU B 171    -7.033  73.952  25.037  1.00 27.92    B   N
ATOM  3340 CA  GLU B 171    -8.117  73.860  24.078  1.00 30.46    B   C
ATOM  3341 CB  GLU B 171    -9.035  72.693  24.435  1.00 34.23    B   C
ATOM  3342 CG  GLU B 171    -8.408  71.310  24.268  1.00 36.53    B   C
ATOM  3343 CD  GLU B 171    -7.963  71.029  22.844  1.00 38.06    B   C
ATOM  3344 OE1 GLU B 171    -8.773  71.218  21.911  1.00 38.60    B   O
ATOM  3345 OE2 GLU B 171    -6.800  70.614  22.659  1.00 38.27    B   O
ATOM  3346 C   GLU B 171    -8.903  75.155  24.104  1.00 30.56    B   C
ATOM  3347 O   GLU B 171    -9.477  75.560  23.093  1.00 33.13    B   O
ATOM  3348 N   ILE B 172    -8.922  75.801  25.265  1.00 27.64    B   N
ATOM  3349 CA  ILE B 172    -9.627  77.060  25.428  1.00 26.46    B   C
ATOM  3350 CB  ILE B 172   -10.239  77.179  26.838  1.00 26.68    B   C
ATOM  3351 CG2 ILE B 172   -10.916  78.534  26.994  1.00 26.23    B   C
ATOM  3352 CG1 ILE B 172   -11.246  76.050  27.071  1.00 27.08    B   C
ATOM  3353 CD1 ILE B 172   -11.899  76.085  28.443  1.00 27.76    B   C
ATOM  3354 C   ILE B 172    -8.670  78.225  25.218  1.00 26.74    B   C
ATOM  3355 O   ILE B 172    -7.604  78.284  25.833  1.00 24.89    B   O
ATOM  3356 N   LEU B 173    -9.055  79.148  24.343  1.00 25.65    B   N
ATOM  3357 CA  LEU B 173    -8.245  80.328  24.061  1.00 25.77    B   C
ATOM  3358 CB  LEU B 173    -8.564  80.853  22.659  1.00 28.20    B   C
ATOM  3359 CG  LEU B 173    -7.682  81.962  22.082  1.00 29.17    B   C
ATOM  3360 CD1 LEU B 173    -6.227  81.521  22.081  1.00 31.35    B   C
ATOM  3361 CD2 LEU B 173    -8.144  82.281  20.661  1.00 29.98    B   C
ATOM  3362 C   LEU B 173    -8.585  81.387  25.111  1.00 24.69    B   C
ATOM  3363 O   LEU B 173    -9.720  81.852  25.188  1.00 26.80    B   O
ATOM  3364 N   PRO B 174    -7.606  81.780  25.939  1.00 21.86    B   N
ATOM  3365 CD  PRO B 174    -6.227  81.269  26.032  1.00 20.12    B   C
ATOM  3366 CA  PRO B 174    -7.857  82.786  26.973  1.00 21.00    B   C
ATOM  3367 CB  PRO B 174    -6.629  82.663  27.873  1.00 20.86    B   C
ATOM  3368 CG  PRO B 174    -5.553  82.313  26.900  1.00 20.88    B   C
ATOM  3369 C   PRO B 174    -8.058  84.215  26.481  1.00 21.07    B   C
ATOM  3370 O   PRO B 174    -7.442  84.652  25.510  1.00 20.92    B   O
ATOM  3371 N   GLU B 175    -8.941  84.932  27.163  1.00 20.88    B   N
ATOM  3372 CA  GLU B 175    -9.210  86.325  26.849  1.00 20.49    B   C
ATOM  3373 CB  GLU B 175   -10.714  86.599  26.886  1.00 22.18    B   C
ATOM  3374 CG  GLU B 175   -11.414  86.262  25.584  1.00 24.72    B   C
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Figure 7HHH

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ATOM  3375 CD  GLU B 175    -12.914  86.445  25.662  1.00 27.87    B   C
ATOM  3376 OE1 GLU B 175    -13.362  87.355  26.386  1.00 29.73    B   O
ATOM  3377 OE2 GLU B 175    -13.643  85.686  24.989  1.00 30.38    B   O
ATOM  3378 C   GLU B 175     -8.492  87.110  27.932  1.00 19.76    B   C
ATOM  3379 O   GLU B 175     -8.151  88.278  27.760  1.00 19.06    B   O
ATOM  3380 N   VAL B 176     -8.249  86.429  29.047  1.00 18.72    B   N
ATOM  3381 CA  VAL B 176     -7.561  87.013  30.187  1.00 18.26    B   C
ATOM  3382 CB  VAL B 176     -8.542  87.366  31.329  1.00 19.04    B   C
ATOM  3383 CG1 VAL B 176     -7.792  88.005  32.473  1.00 17.96    B   C
ATOM  3384 CG2 VAL B 176     -9.627  88.307  30.819  1.00 19.77    B   C
ATOM  3385 C   VAL B 176     -6.566  85.994  30.728  1.00 18.77    B   C
ATOM  3386 O   VAL B 176     -6.909  84.830  30.936  1.00 18.44    B   O
ATOM  3387 N   ILE B 177     -5.337  86.438  30.955  1.00 15.78    B   N
ATOM  3388 CA  ILE B 177     -4.302  85.564  31.485  1.00 15.67    B   C
ATOM  3389 CB  ILE B 177     -3.149  85.366  30.479  1.00 16.57    B   C
ATOM  3390 CG2 ILE B 177     -2.076  84.471  31.092  1.00 15.73    B   C
ATOM  3391 CG1 ILE B 177     -3.679  84.754  29.184  1.00 17.67    B   C
ATOM  3392 CD1 ILE B 177     -2.639  84.634  28.094  1.00 16.12    B   C
ATOM  3393 C   ILE B 177     -3.730  86.191  32.746  1.00 15.83    B   C
ATOM  3394 O   ILE B 177     -3.319  87.356  32.742  1.00 15.47    B   O
ATOM  3395 N   ILE B 178     -3.721  85.427  33.832  1.00 15.84    B   N
ATOM  3396 CA  ILE B 178     -3.178  85.932  35.080  1.00 15.63    B   C
ATOM  3397 CB  ILE B 178     -3.958  85.402  36.314  1.00 16.93    B   C
ATOM  3398 CG2 ILE B 178     -3.370  85.986  37.589  1.00 15.87    B   C
ATOM  3399 CG1 ILE B 178     -5.432  85.807  36.228  1.00 18.02    B   C
ATOM  3400 CD1 ILE B 178     -6.267  85.341  37.422  1.00 17.46    B   C
ATOM  3401 C   ILE B 178     -1.724  85.486  35.190  1.00 14.02    B   C
ATOM  3402 O   ILE B 178     -1.416  84.300  35.089  1.00 13.65    B   O
ATOM  3403 N   LEU B 179     -0.833  86.449  35.376  1.00 14.12    B   N
ATOM  3404 CA  LEU B 179      0.589  86.150  35.525  1.00 14.34    B   C
ATOM  3405 CB  LEU B 179      1.428  87.340  35.053  1.00 15.34    B   C
ATOM  3406 CG  LEU B 179      1.169  87.783  33.610  1.00 16.04    B   C
ATOM  3407 CD1 LEU B 179      1.942  89.073  33.332  1.00 18.24    B   C
ATOM  3408 CD2 LEU B 179      1.574  86.680  32.636  1.00 16.26    B   C
ATOM  3409 C   LEU B 179      0.783  85.915  37.021  1.00 14.01    B   C
ATOM  3410 O   LEU B 179      1.391  86.727  37.719  1.00 13.42    B   O
ATOM  3411 N   GLY B 180      0.252  84.790  37.493  1.00 13.50    B   N
ATOM  3412 CA  GLY B 180      0.310  84.448  38.906  1.00 13.79    B   C
ATOM  3413 C   GLY B 180      1.632  83.927  39.417  1.00 12.30    B   C
ATOM  3414 O   GLY B 180      1.681  82.902  40.093  1.00 14.02    B   O
ATOM  3415 N   CYS B 181      2.702  84.647  39.093  1.00 13.12    B   N
ATOM  3416 CA  CYS B 181      4.048  84.295  39.518  1.00 11.26    B   C
ATOM  3417 CB  CYS B 181      4.591  83.150  38.667  1.00 11.52    B   C
ATOM  3418 SG  CYS B 181      6.279  82.671  39.091  1.00 14.29    B   S
ATOM  3419 C   CYS B 181      4.927  85.532  39.348  1.00 11.67    B   C
ATOM  3420 O   CYS B 181      4.837  86.226  38.336  1.00 10.15    B   O
ATOM  3421 N   THR B 182      5.770  85.796  40.342  1.00 10.95    B   N
ATOM  3422 CA  THR B 182      6.671  86.950  40.329  1.00 11.68    B   C
ATOM  3423 CB  THR B 182      7.654  86.902  41.517  1.00 12.29    B   C
ATOM  3424 OG1 THR B 182      8.306  85.623  41.546  1.00  8.82    B   O
ATOM  3425 CG2 THR B 182      6.918  87.133  42.832  1.00 13.05    B   C
ATOM  3426 C   THR B 182      7.511  87.085  39.068  1.00 12.00    B   C
ATOM  3427 O   THR B 182      7.775  88.190  38.604  1.00 11.14    B   O
ATOM  3428 N   HIS B 183      7.927  85.953  38.516  1.00 11.51    B   N
ATOM  3429 CA  HIS B 183      8.782  85.934  37.333  1.00 12.53    B   C
ATOM  3430 CB  HIS B 183      9.490  84.577  37.250  1.00 12.11    B   C
ATOM  3431 CG  HIS B 183     10.413  84.301  38.396  1.00 12.62    B   C
ATOM  3432 CD2 HIS B 183     11.662  83.774  38.425  1.00 14.37    B   C
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Figure 7III

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ATOM  3433 ND1 HIS B 183    10.074  84.558  39.708  1.00 12.87    B   N
ATOM  3434 CE1 HIS B 183    11.076  84.206  40.495  1.00 11.92    B   C
ATOM  3435 NE2 HIS B 183    12.051  83.728  39.741  1.00 12.64    B   N
ATOM  3436 C   HIS B 183     8.113  86.202  35.990  1.00 13.70    B   C
ATOM  3437 O   HIS B 183     8.735  86.757  35.082  1.00 14.63    B   O
ATOM  3438 N   PHE B 184     6.846  85.822  35.866  1.00 14.67    B   N
ATOM  3439 CA  PHE B 184     6.134  85.945  34.595  1.00 13.80    B   C
ATOM  3440 CB  PHE B 184     4.751  85.298  34.731  1.00 14.23    B   C
ATOM  3441 CG  PHE B 184     4.809  83.829  35.102  1.00 13.65    B   C
ATOM  3442 CD1 PHE B 184     3.646  83.084  35.240  1.00 16.74    B   C
ATOM  3443 CD2 PHE B 184     6.035  83.207  35.355  1.00 14.92    B   C
ATOM  3444 CE1 PHE B 184     3.698  81.743  35.631  1.00 13.35    B   C
ATOM  3445 CE2 PHE B 184     6.097  81.866  35.746  1.00 14.40    B   C
ATOM  3446 CZ  PHE B 184     4.923  81.136  35.884  1.00 13.35    B   C
ATOM  3447 C   PHE B 184     6.049  87.314  33.921  1.00 13.82    B   C
ATOM  3448 O   PHE B 184     5.991  87.391  32.691  1.00 13.30    B   O
ATOM  3449 N   PRO B 185     6.032  88.409  34.697  1.00 13.55    B   N
ATOM  3450 CD  PRO B 185     5.786  88.577  36.143  1.00 14.61    B   C
ATOM  3451 CA  PRO B 185     5.966  89.701  34.008  1.00 14.00    B   C
ATOM  3452 CB  PRO B 185     5.964  90.702  35.158  1.00 15.55    B   C
ATOM  3453 CG  PRO B 185     5.186  89.971  36.210  1.00 16.68    B   C
ATOM  3454 C   PRO B 185     7.158  89.907  33.063  1.00 14.41    B   C
ATOM  3455 O   PRO B 185     7.057  90.640  32.076  1.00 14.66    B   O
ATOM  3456 N   LEU B 186     8.285  89.257  33.355  1.00 13.60    B   N
ATOM  3457 CA  LEU B 186     9.462  89.410  32.503  1.00 14.78    B   C
ATOM  3458 CB  LEU B 186    10.707  88.844  33.185  1.00 16.45    B   C
ATOM  3459 CG  LEU B 186    11.268  89.716  34.312  1.00 17.76    B   C
ATOM  3460 CD1 LEU B 186    12.601  89.149  34.788  1.00 18.57    B   C
ATOM  3461 CD2 LEU B 186    11.454  91.145  33.800  1.00 19.96    B   C
ATOM  3462 C   LEU B 186     9.299  88.796  31.115  1.00 14.26    B   C
ATOM  3463 O   LEU B 186    10.105  89.060  30.219  1.00 13.67    B   O
ATOM  3464 N   ILE B 187     8.271  87.973  30.933  1.00 13.72    B   N
ATOM  3465 CA  ILE B 187     8.007  87.391  29.616  1.00 14.52    B   C
ATOM  3466 CB  ILE B 187     8.252  85.852  29.567  1.00 16.13    B   C
ATOM  3467 CG2 ILE B 187     9.734  85.563  29.730  1.00 15.11    B   C
ATOM  3468 CG1 ILE B 187     7.418  85.134  30.630  1.00 14.95    B   C
ATOM  3469 CD1 ILE B 187     7.386  83.616  30.452  1.00 18.91    B   C
ATOM  3470 C   ILE B 187     6.559  87.681  29.216  1.00 15.97    B   C
ATOM  3471 O   ILE B 187     5.970  86.973  28.399  1.00 14.41    B   O
ATOM  3472 N   ALA B 188     6.003  88.742  29.790  1.00 14.30    B   N
ATOM  3473 CA  ALA B 188     4.623  89.138  29.511  1.00 16.72    B   C
ATOM  3474 CB  ALA B 188     4.261  90.381  30.318  1.00 17.73    B   C
ATOM  3475 C   ALA B 188     4.386  89.386  28.021  1.00 17.75    B   C
ATOM  3476 O   ALA B 188     3.473  88.806  27.437  1.00 15.55    B   O
ATOM  3477 N   GLN B 189     5.208  90.232  27.404  1.00 18.64    B   N
ATOM  3478 CA  GLN B 189     5.045  90.521  25.979  1.00 20.60    B   C
ATOM  3479 CB  GLN B 189     5.977  91.668  25.553  1.00 24.25    B   C
ATOM  3480 CG  GLN B 189     7.448  91.297  25.369  1.00 34.75    B   C
ATOM  3481 CD  GLN B 189     8.385  92.508  25.450  1.00 39.99    B   C
ATOM  3482 OE1 GLN B 189     7.963  93.653  25.263  1.00 43.74    B   O
ATOM  3483 NE2 GLN B 189     9.663  92.254  25.720  1.00 40.19    B   N
ATOM  3484 C   GLN B 189     5.279  89.273  25.111  1.00 17.97    B   C
ATOM  3485 O   GLN B 189     4.729  89.163  24.015  1.00 14.32    B   O
ATOM  3486 N   LYS B 190     6.078  88.329  25.606  1.00 17.40    B   N
ATOM  3487 CA  LYS B 190     6.341  87.097  24.859  1.00 16.80    B   C
ATOM  3488 CB  LYS B 190     7.567  86.374  25.421  1.00 18.22    B   C
ATOM  3489 CG  LYS B 190     8.878  87.117  25.218  1.00 21.88    B   C
ATOM  3490 CD  LYS B 190     9.211  87.269  23.740  1.00 25.45    B   C
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Figure 7JJJ

ATOM 3491 CE LYS B 190 10.416 88.179 23.543 1.00 29.36 B C
ATOM 3492 NZ LYS B 190 10.790 88.298 22.110 1.00 29.28 B N
ATOM 3493 C LYS B 190 5.123 86.176 24.920 1.00 16.76 B C
ATOM 3494 O LYS B 190 4.775 85.521 23.934 1.00 15.72 B O
ATOM 3495 N ILE B 191 4.484 86.118 26.085 1.00 17.36 B N
ATOM 3496 CA ILE B 191 3.293 85.293 26.250 1.00 16.65 B C
ATOM 3497 CB ILE B 191 2.835 85.283 27.722 1.00 16.29 B C
ATOM 3498 CG2 ILE B 191 1.429 84.706 27.837 1.00 15.90 B C
ATOM 3499 CG1 ILE B 191 3.827 84.472 28.561 1.00 14.41 B C
ATOM 3500 CD1 ILE B 191 3.575 84.556 30.065 1.00 15.15 B C
ATOM 3501 C ILE B 191 2.206 85.902 25.371 1.00 17.73 B C
ATOM 3502 O ILE B 191 1.431 85.201 24.730 1.00 17.39 B O
ATOM 3503 N GLU B 192 2.174 87.227 25.343 1.00 19.90 B N
ATOM 3504 CA GLU B 192 1.206 87.955 24.545 1.00 20.35 B C
ATOM 3505 CB GLU B 192 1.368 89.452 24.811 1.00 22.52 B C
ATOM 3506 CG GLU B 192 0.186 90.301 24.426 1.00 31.49 B C
ATOM 3507 CD GLU B 192 0.310 91.705 24.981 1.00 36.51 B C
ATOM 3508 OE1 GLU B 192 0.342 91.845 26.223 1.00 39.33 B O
ATOM 3509 OE2 GLU B 192 0.384 92.660 24.179 1.00 38.77 B O
ATOM 3510 C GLU B 192 1.468 87.638 23.077 1.00 18.85 B C
ATOM 3511 O GLU B 192 0.553 87.274 22.327 1.00 18.00 B O
ATOM 3512 N GLY B 193 2.733 87.764 22.685 1.00 19.26 B N
ATOM 3513 CA GLY B 193 3.134 87.497 21.319 1.00 16.37 B C
ATOM 3514 C GLY B 193 2.843 86.078 20.880 1.00 17.40 B C
ATOM 3515 O GLY B 193 2.580 85.832 19.700 1.00 19.53 B O
ATOM 3516 N TYR B 194 2.892 85.138 21.819 1.00 15.60 B N
ATOM 3517 CA TYR B 194 2.621 83.740 21.494 1.00 16.39 B C
ATOM 3518 CB TYR B 194 2.829 82.845 22.715 1.00 16.47 B C
ATOM 3519 CG TYR B 194 2.502 81.386 22.452 1.00 15.75 B C
ATOM 3520 CD1 TYR B 194 3.470 80.515 21.964 1.00 17.79 B C
ATOM 3521 CE1 TYR B 194 3.171 79.178 21.698 1.00 18.26 B C
ATOM 3522 CD2 TYR B 194 1.216 80.887 22.669 1.00 15.15 B C
ATOM 3523 CE2 TYR B 194 0.904 79.551 22.403 1.00 16.44 B C
ATOM 3524 CZ TYR B 194 1.890 78.703 21.920 1.00 15.60 B C
ATOM 3525 OH TYR B 194 1.614 77.379 21.671 1.00 17.72 B O
ATOM 3526 C TYR B 194 1.189 83.551 21.003 1.00 16.01 B C
ATOM 3527 O TYR B 194 0.966 82.985 19.940 1.00 17.33 B O
ATOM 3528 N PHE B 195 0.218 84.011 21.785 1.00 17.37 B N
ATOM 3529 CA PHE B 195 -1.177 83.851 21.390 1.00 19.84 B C
ATOM 3530 CB PHE B 195 -2.108 84.174 22.563 1.00 20.48 B C
ATOM 3531 CG PHE B 195 -2.057 83.146 23.659 1.00 21.18 B C
ATOM 3532 CD1 PHE B 195 -1.166 83.281 24.720 1.00 20.24 B C
ATOM 3533 CD2 PHE B 195 -2.847 82.002 23.590 1.00 20.40 B C
ATOM 3534 CE1 PHE B 195 -1.061 82.289 25.692 1.00 18.52 B C
ATOM 3535 CE2 PHE B 195 -2.748 81.004 24.558 1.00 21.83 B C
ATOM 3536 CZ PHE B 195 -1.853 81.149 25.609 1.00 18.80 B C
ATOM 3537 C PHE B 195 -1.549 84.675 20.168 1.00 21.22 B C
ATOM 3538 O PHE B 195 -2.381 84.260 19.364 1.00 23.42 B O
ATOM 3539 N MET B 196 -0.920 85.835 20.018 1.00 20.91 B N
ATOM 3540 CA MET B 196 -1.191 86.691 18.874 1.00 22.63 B C
ATOM 3541 CB MET B 196 -0.632 88.096 19.110 1.00 21.19 B C
ATOM 3542 CG MET B 196 -1.454 88.939 20.066 1.00 21.47 B C
ATOM 3543 SD MET B 196 -3.106 89.333 19.420 1.00 22.89 B S
ATOM 3544 CE MET B 196 -2.734 90.738 18.369 1.00 25.90 B C
ATOM 3545 C MET B 196 -0.574 86.098 17.616 1.00 22.76 B C
ATOM 3546 O MET B 196 -1.034 86.365 16.510 1.00 22.32 B O
ATOM 3547 N GLY B 197 0.462 85.284 17.788 1.00 23.35 B N
ATOM 3548 CA GLY B 197 1.117 84.682 16.644 1.00 23.78 B C

Figure 7KKK

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ATOM  3549 C   GLY B 197     0.612  83.294  16.308 1.00 26.07    B   C
ATOM  3550 O   GLY B 197     0.757  82.836  15.178 1.00 27.06    B   O
ATOM  3551 N   HIS B 198     0.011  82.618  17.280 1.00 24.62    B   N
ATOM  3552 CA  HIS B 198    -0.489  81.270  17.052 1.00 25.26    B   C
ATOM  3553 CB  HIS B 198    -0.143  80.393  18.250 1.00 24.79    B   C
ATOM  3554 CG  HIS B 198     1.318  80.087  18.358 1.00 27.65    B   C
ATOM  3555 CD2 HIS B 198     2.369  80.867  18.706 1.00 27.06    B   C
ATOM  3556 ND1 HIS B 198     1.847  78.858  18.026 1.00 29.54    B   N
ATOM  3557 CE1 HIS B 198     3.161  78.896  18.162 1.00 28.74    B   C
ATOM  3558 NE2 HIS B 198     3.503  80.104  18.572 1.00 27.31    B   N
ATOM  3559 C   HIS B 198    -1.982  81.189  16.742 1.00 25.16    B   C
ATOM  3560 O   HIS B 198    -2.470  80.160  16.274 1.00 25.84    B   O
ATOM  3561 N   PHE B 199    -2.701  82.274  17.002 1.00 23.99    B   N
ATOM  3562 CA  PHE B 199    -4.134  82.323  16.731 1.00 25.24    B   C
ATOM  3563 CB  PHE B 199    -4.939  82.150  18.021 1.00 25.35    B   C
ATOM  3564 CG  PHE B 199    -4.641  80.875  18.754 1.00 25.83    B   C
ATOM  3565 CD1 PHE B 199    -3.499  80.763  19.543 1.00 25.81    B   C
ATOM  3566 CD2 PHE B 199    -5.486  79.776  18.634 1.00 26.63    B   C
ATOM  3567 CE1 PHE B 199    -3.202  79.571  20.204 1.00 25.90    B   C
ATOM  3568 CE2 PHE B 199    -5.200  78.574  19.292 1.00 27.07    B   C
ATOM  3569 CZ  PHE B 199    -4.053  78.476  20.078 1.00 25.59    B   C
ATOM  3570 C   PHE B 199    -4.488  83.658  16.085 1.00 25.45    B   C
ATOM  3571 O   PHE B 199    -3.741  84.633  16.202 1.00 26.05    B   O
ATOM  3572 N   ALA B 200    -5.624  83.698  15.397 1.00 25.36    B   N
ATOM  3573 CA  ALA B 200    -6.066  84.926  14.744 1.00 26.49    B   C
ATOM  3574 CB  ALA B 200    -6.945  84.592  13.543 1.00 27.04    B   C
ATOM  3575 C   ALA B 200    -6.842  85.770  15.748 1.00 25.75    B   C
ATOM  3576 O   ALA B 200    -8.035  85.555  15.951 1.00 27.07    B   O
ATOM  3577 N   LEU B 201    -6.162  86.723  16.380 1.00 26.03    B   N
ATOM  3578 CA  LEU B 201    -6.801  87.588  17.371 1.00 25.45    B   C
ATOM  3579 CB  LEU B 201    -6.206  87.345  18.762 1.00 26.37    B   C
ATOM  3580 CG  LEU B 201    -6.409  85.971  19.404 1.00 27.87    B   C
ATOM  3581 CD1 LEU B 201    -5.727  85.944  20.768 1.00 27.55    B   C
ATOM  3582 CD2 LEU B 201    -7.895  85.681  19.539 1.00 28.11    B   C
ATOM  3583 C   LEU B 201    -6.668  89.069  17.041 1.00 24.86    B   C
ATOM  3584 O   LEU B 201    -5.571  89.565  16.801 1.00 25.77    B   O
ATOM  3585 N   PRO B 202    -7.792  89.795  17.036 1.00 25.07    B   N
ATOM  3586 CD  PRO B 202    -9.159  89.302  17.284 1.00 27.27    B   C
ATOM  3587 CA  PRO B 202    -7.801  91.229  16.739 1.00 27.30    B   C
ATOM  3588 CB  PRO B 202    -9.286  91.530  16.571 1.00 26.61    B   C
ATOM  3589 CG  PRO B 202    -9.919  90.581  17.541 1.00 28.74    B   C
ATOM  3590 C   PRO B 202    -7.162  92.024  17.878 1.00 28.85    B   C
ATOM  3591 O   PRO B 202    -6.625  93.111  17.676 1.00 31.54    B   O
ATOM  3592 N   THR B 203    -7.228  91.467  19.080 1.00 29.83    B   N
ATOM  3593 CA  THR B 203    -6.649  92.104  20.253 1.00 30.73    B   C
ATOM  3594 CB  THR B 203    -7.717  92.910  21.029 1.00 32.69    B   C
ATOM  3595 OG1 THR B 203    -7.113  93.535  22.168 1.00 38.76    B   O
ATOM  3596 CG2 THR B 203    -8.854  92.009  21.478 1.00 34.49    B   C
ATOM  3597 C   THR B 203    -6.057  91.009  21.142 1.00 30.11    B   C
ATOM  3598 O   THR B 203    -6.632  89.929  21.281 1.00 29.77    B   O
ATOM  3599 N   PRO B 204    -4.888  91.271  21.746 1.00 28.28    B   N
ATOM  3600 CD  PRO B 204    -4.105  92.519  21.714 1.00 29.99    B   C
ATOM  3601 CA  PRO B 204    -4.249  90.278  22.608 1.00 25.72    B   C
ATOM  3602 CB  PRO B 204    -2.871  90.878  22.851 1.00 27.64    B   C
ATOM  3603 CG  PRO B 204    -3.170  92.344  22.895 1.00 30.54    B   C
ATOM  3604 C   PRO B 204    -5.007  90.034  23.906 1.00 22.99    B   C
ATOM  3605 O   PRO B 204    -5.829  90.847  24.322 1.00 21.45    B   O
ATOM  3606 N   PRO B 205    -4.754  88.888  24.550 1.00 23.17    B   N
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Figure 7LLL

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ATOM  3607 CD  PRO B 205     -3.967  87.734  24.079  1.00 22.14    B   C
ATOM  3608 CA  PRO B 205     -5.435  88.579  25.812  1.00 21.71    B   C
ATOM  3609 CB  PRO B 205     -4.930  87.177  26.145  1.00 20.02    B   C
ATOM  3610 CG  PRO B 205     -4.640  86.587  24.791  1.00 24.28    B   C
ATOM  3611 C   PRO B 205     -5.013  89.592  26.870  1.00 20.42    B   C
ATOM  3612 O   PRO B 205     -3.884  90.081  26.855  1.00 20.68    B   O
ATOM  3613 N   LEU B 206     -5.920  89.912  27.781  1.00 19.56    B   N
ATOM  3614 CA  LEU B 206     -5.614  90.852  28.844  1.00 18.19    B   C
ATOM  3615 CB  LEU B 206     -6.903  91.341  29.506  1.00 19.98    B   C
ATOM  3616 CG  LEU B 206     -6.733  92.187  30.772  1.00 20.16    B   C
ATOM  3617 CD1 LEU B 206     -6.025  93.490  30.435  1.00 20.32    B   C
ATOM  3618 CD2 LEU B 206     -8.097  92.461  31.383  1.00 21.77    B   C
ATOM  3619 C   LEU B 206     -4.748  90.152  29.887  1.00 19.09    B   C
ATOM  3620 O   LEU B 206     -5.155  89.137  30.460  1.00 16.01    B   O
ATOM  3621 N   LEU B 207     -3.554  90.682  30.130  1.00 17.87    B   N
ATOM  3622 CA  LEU B 207     -2.673  90.086  31.128  1.00 19.96    B   C
ATOM  3623 CB  LEU B 207     -1.204  90.137  30.683  1.00 20.75    B   C
ATOM  3624 CG  LEU B 207     -0.775  89.375  29.427  1.00 23.64    B   C
ATOM  3625 CD1 LEU B 207      0.754  89.247  29.409  1.00 24.69    B   C
ATOM  3626 CD2 LEU B 207     -1.402  88.003  29.411  1.00 25.49    B   C
ATOM  3627 C   LEU B 207     -2.822  90.826  32.450  1.00 18.55    B   C
ATOM  3628 O   LEU B 207     -2.846  92.056  32.489  1.00 19.17    B   O
ATOM  3629 N   ILE B 208     -2.925  90.067  33.534  1.00 17.96    B   N
ATOM  3630 CA  ILE B 208     -3.064  90.645  34.860  1.00 17.50    B   C
ATOM  3631 CB  ILE B 208     -4.118  89.878  35.685  1.00 17.43    B   C
ATOM  3632 CG2 ILE B 208     -4.243  90.491  37.077  1.00 18.18    B   C
ATOM  3633 CG1 ILE B 208     -5.459  89.892  34.943  1.00 18.45    B   C
ATOM  3634 CD1 ILE B 208     -6.012  91.289  34.699  1.00 14.50    B   C
ATOM  3635 C   ILE B 208     -1.719  90.585  35.575  1.00 16.82    B   C
ATOM  3636 O   ILE B 208     -1.164  89.508  35.780  1.00 15.89    B   O
ATOM  3637 N   HIS B 209     -1.213  91.756  35.950  1.00 17.14    B   N
ATOM  3638 CA  HIS B 209      0.074  91.899  36.632  1.00 18.16    B   C
ATOM  3639 CB  HIS B 209      0.745  93.175  36.106  1.00 18.91    B   C
ATOM  3640 CG  HIS B 209      2.193  93.306  36.457  1.00 20.99    B   C
ATOM  3641 CD2 HIS B 209      3.306  93.162  35.699  1.00 19.36    B   C
ATOM  3642 ND1 HIS B 209      2.629  93.657  37.716  1.00 22.36    B   N
ATOM  3643 CE1 HIS B 209      3.949  93.725  37.718  1.00 21.52    B   C
ATOM  3644 NE2 HIS B 209      4.384  93.429  36.506  1.00 15.94    B   N
ATOM  3645 C   HIS B 209     -0.149  91.980  38.150  1.00 17.31    B   C
ATOM  3646 O   HIS B 209     -0.909  92.826  38.621  1.00 17.80    B   O
ATOM  3647 N   SER B 210      0.513  91.104  38.908  1.00 15.90    B   N
ATOM  3648 CA  SER B 210      0.361  91.070  40.366  1.00 18.09    B   C
ATOM  3649 CB  SER B 210      1.187  89.931  40.975  1.00 15.92    B   C
ATOM  3650 OG  SER B 210      0.783  88.671  40.475  1.00 17.30    B   O
ATOM  3651 C   SER B 210      0.762  92.368  41.048  1.00 18.89    B   C
ATOM  3652 O   SER B 210      0.146  92.783  42.036  1.00 18.64    B   O
ATOM  3653 N   GLY B 211      1.806  92.999  40.527  1.00 18.49    B   N
ATOM  3654 CA  GLY B 211      2.276  94.241  41.105  1.00 17.93    B   C
ATOM  3655 C   GLY B 211      1.300  95.384  40.929  1.00 18.65    B   C
ATOM  3656 O   GLY B 211      0.988  96.088  41.888  1.00 18.89    B   O
ATOM  3657 N   ASP B 212      0.821  95.585  39.708  1.00 17.89    B   N
ATOM  3658 CA  ASP B 212     -0.122  96.666  39.454  1.00 19.78    B   C
ATOM  3659 CB  ASP B 212     -0.441  96.776  37.959  1.00 21.36    B   C
ATOM  3660 CG  ASP B 212      0.789  97.074  37.119  1.00 25.55    B   C
ATOM  3661 OD1 ASP B 212      1.588  97.954  37.509  1.00 24.93    B   O
ATOM  3662 OD2 ASP B 212      0.948  96.432  36.059  1.00 27.71    B   O
ATOM  3663 C   ASP B 212     -1.414  96.441  40.227  1.00 18.76    B   C
ATOM  3664 O   ASP B 212     -2.025  97.389  40.712  1.00 19.27    B   O
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Figure 7MMM

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ATOM  3665 N   ALA B 213    -1.825  95.182  40.344  1.00 19.86    B   N
ATOM  3666 CA  ALA B 213    -3.055  94.847  41.054  1.00 17.54    B   C
ATOM  3667 CB  ALA B 213    -3.378  93.372  40.876  1.00 17.05    B   C
ATOM  3668 C   ALA B 213    -2.959  95.183  42.539  1.00 19.06    B   C
ATOM  3669 O   ALA B 213    -3.901  95.725  43.120  1.00 16.90    B   O
ATOM  3670 N   ILE B 214    -1.823  94.876  43.158  1.00 15.97    B   N
ATOM  3671 CA  ILE B 214    -1.678  95.162  44.577  1.00 16.41    B   C
ATOM  3672 CB  ILE B 214    -0.503  94.357  45.206  1.00 17.51    B   C
ATOM  3673 CG2 ILE B 214     0.841  94.960  44.809  1.00 16.99    B   C
ATOM  3674 CG1 ILE B 214    -0.639  94.359  46.733  1.00 17.48    B   C
ATOM  3675 CD1 ILE B 214     0.283  93.366  47.436  1.00 20.67    B   C
ATOM  3676 C   ILE B 214    -1.516  96.656  44.864  1.00 16.49    B   C
ATOM  3677 O   ILE B 214    -1.933  97.133  45.917  1.00 16.10    B   O
ATOM  3678 N   VAL B 215    -0.927  97.403  43.933  1.00 16.36    B   N
ATOM  3679 CA  VAL B 215    -0.772  98.841  44.139  1.00 17.16    B   C
ATOM  3680 CB  VAL B 215    -0.016  99.509  42.964  1.00 19.48    B   C
ATOM  3681 CG1 VAL B 215    -0.179 101.017  43.027  1.00 17.77    B   C
ATOM  3682 CG2 VAL B 215     1.470  99.147  43.022  1.00 17.10    B   C
ATOM  3683 C   VAL B 215    -2.161  99.471  44.259  1.00 18.05    B   C
ATOM  3684 O   VAL B 215    -2.417 100.282  45.153  1.00 17.39    B   O
ATOM  3685 N   GLU B 216    -3.054  99.089  43.354  1.00 19.67    B   N
ATOM  3686 CA  GLU B 216    -4.411  99.617  43.357  1.00 21.54    B   C
ATOM  3687 CB  GLU B 216    -5.188  99.059  42.166  1.00 23.84    B   C
ATOM  3688 CG  GLU B 216    -4.815  99.727  40.853  1.00 26.87    B   C
ATOM  3689 CD  GLU B 216    -5.388  99.014  39.648  1.00 30.91    B   C
ATOM  3690 OE1 GLU B 216    -5.399  99.623  38.558  1.00 34.30    B   O
ATOM  3691 OE2 GLU B 216    -5.815  97.845  39.785  1.00 31.99    B   O
ATOM  3692 C   GLU B 216    -5.126  99.293  44.657  1.00 20.92    B   C
ATOM  3693 O   GLU B 216    -5.815 100.141  45.223  1.00 19.64    B   O
ATOM  3694 N   TYR B 217    -4.955  98.065  45.135  1.00 21.71    B   N
ATOM  3695 CA  TYR B 217    -5.583  97.649  46.386  1.00 21.99    B   C
ATOM  3696 CB  TYR B 217    -5.307  96.167  46.658  1.00 22.18    B   C
ATOM  3697 CG  TYR B 217    -5.831  95.693  47.995  1.00 20.53    B   C
ATOM  3698 CD1 TYR B 217    -7.199  95.534  48.213  1.00 22.61    B   C
ATOM  3699 CE1 TYR B 217    -7.692  95.113  49.456  1.00 20.09    B   C
ATOM  3700 CD2 TYR B 217    -4.961  95.422  49.051  1.00 19.57    B   C
ATOM  3701 CE2 TYR B 217    -5.440  95.002  50.293  1.00 19.82    B   C
ATOM  3702 CZ  TYR B 217    -6.807  94.849  50.488  1.00 20.38    B   C
ATOM  3703 OH  TYR B 217    -7.288  94.422  51.709  1.00 19.08    B   O
ATOM  3704 C   TYR B 217    -5.056  98.473  47.558  1.00 22.00    B   C
ATOM  3705 O   TYR B 217    -5.832  98.992  48.362  1.00 21.85    B   O
ATOM  3706 N   LEU B 218    -3.734  98.591  47.654  1.00 19.08    B   N
ATOM  3707 CA  LEU B 218    -3.113  99.341  48.740  1.00 19.40    B   C
ATOM  3708 CB  LEU B 218    -1.585  99.279  48.615  1.00 17.82    B   C
ATOM  3709 CG  LEU B 218    -0.941  97.888  48.742  1.00 18.28    B   C
ATOM  3710 CD1 LEU B 218     0.541  97.968  48.389  1.00 15.96    B   C
ATOM  3711 CD2 LEU B 218    -1.128  97.353  50.155  1.00 16.26    B   C
ATOM  3712 C   LEU B 218    -3.582 100.798  48.791  1.00 21.94    B   C
ATOM  3713 O   LEU B 218    -3.841 101.335  49.866  1.00 18.51    B   O
ATOM  3714 N   GLN B 219    -3.691 101.433  47.629  1.00 22.92    B   N
ATOM  3715 CA  GLN B 219    -4.139 102.822  47.562  1.00 24.80    B   C
ATOM  3716 CB  GLN B 219    -4.004 103.353  46.129  1.00 26.04    B   C
ATOM  3717 CG  GLN B 219    -2.577 103.325  45.592  1.00 28.25    B   C
ATOM  3718 CD  GLN B 219    -2.470 103.820  44.156  1.00 28.07    B   C
ATOM  3719 OE1 GLN B 219    -3.166 103.334  43.262  1.00 25.98    B   O
ATOM  3720 NE2 GLN B 219    -1.588 104.790  43.932  1.00 30.48    B   N
ATOM  3721 C   GLN B 219    -5.596 102.914  48.005  1.00 24.27    B   C
ATOM  3722 O   GLN B 219    -5.995 103.859  48.683  1.00 25.16    B   O
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Figure 7NNN

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ATOM  3723  N   GLN B 220     -6.375 101.912  47.620  1.00 24.30      B   N
ATOM  3724  CA  GLN B 220     -7.792 101.838  47.943  1.00 28.00      B   C
ATOM  3725  CB  GLN B 220     -8.410 100.663  47.184  1.00 31.02      B   C
ATOM  3726  CG  GLN B 220     -9.920 100.674  47.077  1.00 39.36      B   C
ATOM  3727  CD  GLN B 220    -10.411 101.639  46.020  1.00 44.14      B   C
ATOM  3728  OE1 GLN B 220    -10.260 102.854  46.154  1.00 47.44      B   O
ATOM  3729  NE2 GLN B 220    -10.995 101.101  44.954  1.00 47.51      B   N
ATOM  3730  C   GLN B 220     -8.013 101.635  49.444  1.00 29.46      B   C
ATOM  3731  O   GLN B 220     -8.553 102.499  50.137  1.00 28.33      B   O
ATOM  3732  N   LYS B 221     -7.570 100.477  49.927  1.00 29.84      B   N
ATOM  3733  CA  LYS B 221     -7.720 100.075  51.321  1.00 28.05      B   C
ATOM  3734  CB  LYS B 221     -7.249  98.626  51.477  1.00 29.20      B   C
ATOM  3735  CG  LYS B 221     -8.124  97.761  52.381  1.00 33.06      B   C
ATOM  3736  CD  LYS B 221     -8.114  98.242  53.817  1.00 34.46      B   C
ATOM  3737  CE  LYS B 221     -8.796  97.239  54.738  1.00 34.63      B   C
ATOM  3738  NZ  LYS B 221     -8.003  95.993  54.896  1.00 31.31      B   N
ATOM  3739  C   LYS B 221     -7.012 100.953  52.345  1.00 27.08      B   C
ATOM  3740  O   LYS B 221     -7.556 101.230  53.416  1.00 27.24      B   O
ATOM  3741  N   TYR B 222     -5.804 101.399  52.029  1.00 25.82      B   N
ATOM  3742  CA  TYR B 222     -5.052 102.212  52.973  1.00 27.04      B   C
ATOM  3743  CB  TYR B 222     -3.658 101.616  53.147  1.00 22.44      B   C
ATOM  3744  CG  TYR B 222     -3.708 100.166  53.576  1.00 22.86      B   C
ATOM  3745  CD1 TYR B 222     -4.156  99.815  54.854  1.00 19.32      B   C
ATOM  3746  CE1 TYR B 222     -4.258  98.484  55.243  1.00 19.44      B   C
ATOM  3747  CD2 TYR B 222     -3.357  99.134  52.694  1.00 20.72      B   C
ATOM  3748  CE2 TYR B 222     -3.456  97.792  53.078  1.00 19.21      B   C
ATOM  3749  CZ  TYR B 222     -3.909  97.482  54.351  1.00 19.82      B   C
ATOM  3750  OH  TYR B 222     -4.027  96.167  54.725  1.00 19.05      B   O
ATOM  3751  C   TYR B 222     -4.968 103.667  52.539  1.00 29.48      B   C
ATOM  3752  O   TYR B 222     -4.096 104.405  52.986  1.00 31.72      B   O
ATOM  3753  N   ALA B 223     -5.900 104.089  51.696  1.00 32.87      B   N
ATOM  3754  CA  ALA B 223     -5.895 105.466  51.201  1.00 36.60      B   C
ATOM  3755  CB  ALA B 223     -6.672 106.421  52.148  1.00 37.41      B   C
ATOM  3756  C   ALA B 223     -4.442 105.909  51.088  1.00 38.06      B   C
ATOM  3757  O   ALA B 223     -4.060 106.977  51.560  1.00 38.78      B   O
ATOM  3758  N   LEU B 224     -3.627 105.088  50.441  1.00 38.57      B   N
ATOM  3759  CA  LEU B 224     -2.215 105.403  50.264  1.00 38.61      B   C
ATOM  3760  CB  LEU B 224     -1.402 104.097  50.136  1.00 39.37      B   C
ATOM  3761  CG  LEU B 224     -1.183 103.355  51.466  1.00 39.96      B   C
ATOM  3762  CD1 LEU B 224     -0.057 102.350  51.297  1.00 39.16      B   C
ATOM  3763  CD2 LEU B 224     -0.818 104.336  52.585  1.00 41.79      B   C
ATOM  3764  C   LEU B 224     -1.949 106.306  49.064  1.00 38.91      B   C
ATOM  3765  O   LEU B 224     -2.714 106.190  48.105  1.00 38.22      B   O
ATOM  3766  OXT LEU B 224     -0.969 107.085  49.068  1.00 39.30      B   O
ATOM  3767  CB  PRO B 232     11.684 106.007  48.754  1.00 35.25      B   C
ATOM  3768  CG  PRO B 232     11.385 107.285  47.963  1.00 36.48      B   C
ATOM  3769  C   PRO B 232     13.583 105.559  50.328  1.00 32.21      B   C
ATOM  3770  O   PRO B 232     14.407 105.139  49.517  1.00 33.63      B   O
ATOM  3771  N   PRO B 232     13.132 107.820  49.423  1.00 34.70      B   N
ATOM  3772  CD  PRO B 232     12.673 108.108  48.053  1.00 35.80      B   C
ATOM  3773  CA  PRO B 232     12.514 106.559  49.903  1.00 34.68      B   C
ATOM  3774  N   LYS B 233     13.566 105.183  51.602  1.00 30.94      B   N
ATOM  3775  CA  LYS B 233     14.542 104.237  52.126  1.00 27.68      B   C
ATOM  3776  CB  LYS B 233     14.693 104.412  53.637  1.00 30.73      B   C
ATOM  3777  CG  LYS B 233     15.074 105.817  54.076  1.00 37.18      B   C
ATOM  3778  CD  LYS B 233     15.073 105.930  55.594  1.00 41.29      B   C
ATOM  3779  CE  LYS B 233     15.358 107.357  56.045  1.00 46.10      B   C
ATOM  3780  NZ  LYS B 233     15.389 107.476  57.535  1.00 49.46      B   N
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Figure 7OOO

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ATOM  3781  C   LYS B 233     14.115 102.805  51.823  1.00 25.78      B   C
ATOM  3782  O   LYS B 233     12.984 102.404  52.108  1.00 21.74      B   O
ATOM  3783  N   VAL B 234     15.027 102.041  51.238  1.00 23.23      B   N
ATOM  3784  CA  VAL B 234     14.755 100.652  50.902  1.00 22.01      B   C
ATOM  3785  CB  VAL B 234     14.425 100.486  49.403  1.00 22.47      B   C
ATOM  3786  CG1 VAL B 234     14.095  99.034  49.105  1.00 23.89      B   C
ATOM  3787  CG2 VAL B 234     13.267 101.386  49.015  1.00 24.31      B   C
ATOM  3788  C   VAL B 234     15.997  99.825  51.204  1.00 21.91      B   C
ATOM  3789  O   VAL B 234     17.083 100.121  50.702  1.00 19.49      B   O
ATOM  3790  N   GLU B 235     15.850  98.805  52.041  1.00 19.26      B   N
ATOM  3791  CA  GLU B 235     16.987  97.956  52.343  1.00 19.57      B   C
ATOM  3792  CB  GLU B 235     17.407  98.085  53.812  1.00 22.19      B   C
ATOM  3793  CG  GLU B 235     16.367  97.736  54.849  1.00 27.30      B   C
ATOM  3794  CD  GLU B 235     16.893  97.954  56.266  1.00 31.20      B   C
ATOM  3795  OE1 GLU B 235     17.214  99.113  56.617  1.00 30.91      B   O
ATOM  3796  OE2 GLU B 235     16.992  96.967  57.027  1.00 31.05      B   O
ATOM  3797  C   GLU B 235     16.667  96.513  51.979  1.00 17.90      B   C
ATOM  3798  O   GLU B 235     15.514  96.071  52.067  1.00 17.20      B   O
ATOM  3799  N   PHE B 236     17.694  95.797  51.538  1.00 15.16      B   N
ATOM  3800  CA  PHE B 236     17.540  94.417  51.121  1.00 14.57      B   C
ATOM  3801  CB  PHE B 236     18.080  94.240  49.702  1.00 13.24      B   C
ATOM  3802  CG  PHE B 236     17.406  95.123  48.695  1.00 14.78      B   C
ATOM  3803  CD1 PHE B 236     17.807  96.448  48.529  1.00 13.54      B   C
ATOM  3804  CD2 PHE B 236     16.338  94.647  47.944  1.00 13.10      B   C
ATOM  3805  CE1 PHE B 236     17.148  97.281  47.625  1.00 15.52      B   C
ATOM  3806  CE2 PHE B 236     15.676  95.471  47.043  1.00 11.79      B   C
ATOM  3807  CZ  PHE B 236     16.083  96.792  46.884  1.00 13.41      B   C
ATOM  3808  C   PHE B 236     18.206  93.432  52.055  1.00 14.79      B   C
ATOM  3809  O   PHE B 236     19.298  93.668  52.566  1.00 14.15      B   O
ATOM  3810  N   HIS B 237     17.519  92.319  52.270  1.00 13.68      B   N
ATOM  3811  CA  HIS B 237     17.993  91.266  53.147  1.00 11.28      B   C
ATOM  3812  CB  HIS B 237     17.235  91.319  54.466  1.00 12.27      B   C
ATOM  3813  CG  HIS B 237     17.437  92.597  55.219  1.00 14.02      B   C
ATOM  3814  CD2 HIS B 237     16.779  93.778  55.159  1.00 14.88      B   C
ATOM  3815  ND1 HIS B 237     18.460  92.771  56.126  1.00 14.41      B   N
ATOM  3816  CE1 HIS B 237     18.423  94.006  56.593  1.00 18.35      B   C
ATOM  3817  NE2 HIS B 237     17.413  94.638  56.023  1.00 14.90      B   N
ATOM  3818  C   HIS B 237     17.705  89.961  52.437  1.00 13.01      B   C
ATOM  3819  O   HIS B 237     16.725  89.860  51.702  1.00 12.07      B   O
ATOM  3820  N   ALA B 238     18.554  88.967  52.665  1.00 12.63      B   N
ATOM  3821  CA  ALA B 238     18.387  87.671  52.022  1.00 11.54      B   C
ATOM  3822  CB  ALA B 238     19.018  87.700  50.639  1.00  9.85      B   C
ATOM  3823  C   ALA B 238     19.010  86.554  52.836  1.00 14.48      B   C
ATOM  3824  O   ALA B 238     19.998  86.765  53.533  1.00 14.69      B   O
ATOM  3825  N   SER B 239     18.424  85.364  52.741  1.00 14.68      B   N
ATOM  3826  CA  SER B 239     18.948  84.202  53.447  1.00 14.80      B   C
ATOM  3827  CB  SER B 239     17.862  83.141  53.608  1.00 13.43      B   C
ATOM  3828  OG  SER B 239     17.340  82.758  52.355  1.00 13.26      B   O
ATOM  3829  C   SER B 239     20.104  83.656  52.614  1.00 14.91      B   C
ATOM  3830  O   SER B 239     20.945  82.902  53.107  1.00 12.99      B   O
ATOM  3831  N   GLY B 240     20.134  84.050  51.344  1.00 14.12      B   N
ATOM  3832  CA  GLY B 240     21.197  83.631  50.455  1.00 15.59      B   C
ATOM  3833  C   GLY B 240     22.217  84.752  50.346  1.00 16.66      B   C
ATOM  3834  O   GLY B 240     22.520  85.416  51.334  1.00 16.99      B   O
ATOM  3835  N   ASP B 241     22.732  84.985  49.145  1.00 15.94      B   N
ATOM  3836  CA  ASP B 241     23.722  86.036  48.947  1.00 17.18      B   C
ATOM  3837  CB  ASP B 241     24.487  85.795  47.649  1.00 18.32      B   C
ATOM  3838  CG  ASP B 241     25.703  86.673  47.527  1.00 21.73      B   C
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Figure 7PPP

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ATOM  3839 OD1 ASP B 241     25.702  87.771  48.126  1.00 22.80    B   O
ATOM  3840 OD2 ASP B 241     26.653  86.277  46.824  1.00 23.86    B   O
ATOM  3841 C   ASP B 241     23.070  87.416  48.899  1.00 15.91    B   C
ATOM  3842 O   ASP B 241     22.566  87.838  47.855  1.00 18.69    B   O
ATOM  3843 N   VAL B 242     23.091  88.125  50.022  1.00 15.82    B   N
ATOM  3844 CA  VAL B 242     22.480  89.447  50.079  1.00 15.47    B   C
ATOM  3845 CB  VAL B 242     22.373  89.961  51.538  1.00 14.55    B   C
ATOM  3846 CG1 VAL B 242     23.753  90.329  52.079  1.00 14.67    B   C
ATOM  3847 CG2 VAL B 242     21.405  91.147  51.599  1.00 13.95    B   C
ATOM  3848 C   VAL B 242     23.230  90.480  49.242  1.00 16.20    B   C
ATOM  3849 O   VAL B 242     22.624  91.396  48.693  1.00 16.97    B   O
ATOM  3850 N   ILE B 243     24.546  90.347  49.145  1.00 15.87    B   N
ATOM  3851 CA  ILE B 243     25.307  91.303  48.351  1.00 15.88    B   C
ATOM  3852 CB  ILE B 243     26.833  91.076  48.512  1.00 17.32    B   C
ATOM  3853 CG2 ILE B 243     27.606  91.924  47.510  1.00 17.19    B   C
ATOM  3854 CG1 ILE B 243     27.249  91.447  49.940  1.00 19.37    B   C
ATOM  3855 CD1 ILE B 243     28.685  91.096  50.286  1.00 19.42    B   C
ATOM  3856 C   ILE B 243     24.882  91.191  46.889  1.00 14.23    B   C
ATOM  3857 O   ILE B 243     24.745  92.200  46.201  1.00 14.19    B   O
ATOM  3858 N   TRP B 244     24.651  89.967  46.421  1.00 14.60    B   N
ATOM  3859 CA  TRP B 244     24.207  89.756  45.046  1.00 14.98    B   C
ATOM  3860 CB  TRP B 244     24.078  88.264  44.729  1.00 15.60    B   C
ATOM  3861 CG  TRP B 244     23.575  87.999  43.329  1.00 16.65    B   C
ATOM  3862 CD2 TRP B 244     22.210  87.806  42.930  1.00 19.35    B   C
ATOM  3863 CE2 TRP B 244     22.206  87.617  41.527  1.00 18.45    B   C
ATOM  3864 CE3 TRP B 244     20.989  87.775  43.622  1.00 18.90    B   C
ATOM  3865 CD1 TRP B 244     24.321  87.924  42.184  1.00 18.57    B   C
ATOM  3866 NE1 TRP B 244     23.506  87.694  41.097  1.00 17.92    B   N
ATOM  3867 CZ2 TRP B 244     21.029  87.398  40.803  1.00 17.47    B   C
ATOM  3868 CZ3 TRP B 244     19.818  87.558  42.902  1.00 18.34    B   C
ATOM  3869 CH2 TRP B 244     19.847  87.371  41.504  1.00 17.51    B   C
ATOM  3870 C   TRP B 244     22.845  90.409  44.850  1.00 16.58    B   C
ATOM  3871 O   TRP B 244     22.616  91.102  43.859  1.00 17.56    B   O
ATOM  3872 N   LEU B 245     21.937  90.180  45.796  1.00 15.30    B   N
ATOM  3873 CA  LEU B 245     20.599  90.749  45.707  1.00 15.38    B   C
ATOM  3874 CB  LEU B 245     19.746  90.306  46.900  1.00 14.42    B   C
ATOM  3875 CG  LEU B 245     18.287  90.782  46.894  1.00 12.51    B   C
ATOM  3876 CD1 LEU B 245     17.536  90.163  45.723  1.00 15.01    B   C
ATOM  3877 CD2 LEU B 245     17.618  90.397  48.215  1.00 15.46    B   C
ATOM  3878 C   LEU B 245     20.648  92.270  45.660  1.00 15.93    B   C
ATOM  3879 O   LEU B 245     19.895  92.901  44.916  1.00 11.84    B   O
ATOM  3880 N   GLU B 246     21.534  92.865  46.454  1.00 16.60    B   N
ATOM  3881 CA  GLU B 246     21.636  94.317  46.480  1.00 17.29    B   C
ATOM  3882 CB  GLU B 246     22.496  94.782  47.658  1.00 18.17    B   C
ATOM  3883 CG  GLU B 246     21.896  94.455  49.020  1.00 19.87    B   C
ATOM  3884 CD  GLU B 246     22.776  94.908  50.176  1.00 21.82    B   C
ATOM  3885 OE1 GLU B 246     24.001  94.687  50.101  1.00 23.59    B   O
ATOM  3886 OE2 GLU B 246     22.244  95.471  51.161  1.00 18.84    B   O
ATOM  3887 C   GLU B 246     22.213  94.819  45.171  1.00 19.10    B   C
ATOM  3888 O   GLU B 246     21.866  95.905  44.711  1.00 18.10    B   O
ATOM  3889 N   ARG B 247     23.082  94.016  44.564  1.00 20.90    B   N
ATOM  3890 CA  ARG B 247     23.694  94.384  43.296  1.00 21.36    B   C
ATOM  3891 CB  ARG B 247     24.819  93.407  42.945  1.00 23.57    B   C
ATOM  3892 CG  ARG B 247     25.698  93.843  41.780  1.00 28.81    B   C
ATOM  3893 CD  ARG B 247     26.796  92.813  41.516  1.00 31.64    B   C
ATOM  3894 NE  ARG B 247     27.648  92.622  42.688  1.00 33.01    B   N
ATOM  3895 CZ  ARG B 247     27.953  91.437  43.214  1.00 34.15    B   C
ATOM  3896 NH1 ARG B 247     27.475  90.319  42.678  1.00 32.31    B   N
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Figure 7QQQ

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ATOM  3897 NH2 ARG B 247     28.742  91.372  44.281  1.00 32.59      B   N
ATOM  3898 C   ARG B 247     22.612  94.369  42.218  1.00 21.28      B   C
ATOM  3899 O   ARG B 247     22.613  95.212  41.319  1.00 18.68      B   O
ATOM  3900 N   GLN B 248     21.689  93.411  42.316  1.00 19.88      B   N
ATOM  3901 CA  GLN B 248     20.587  93.310  41.359  1.00 18.33      B   C
ATOM  3902 CB  GLN B 248     19.778  92.027  41.586  1.00 16.87      B   C
ATOM  3903 CG  GLN B 248     20.458  90.749  41.119  1.00 17.30      B   C
ATOM  3904 CD  GLN B 248     20.794  90.768  39.631  1.00 21.87      B   C
ATOM  3905 OE1 GLN B 248     19.946  91.077  38.790  1.00 23.30      B   O
ATOM  3906 NE2 GLN B 248     22.032  90.423  39.304  1.00 24.03      B   N
ATOM  3907 C   GLN B 248     19.670  94.518  41.528  1.00 17.34      B   C
ATOM  3908 O   GLN B 248     19.166  95.071  40.550  1.00 16.87      B   O
ATOM  3909 N   ALA B 249     19.451  94.917  42.777  1.00 15.06      B   N
ATOM  3910 CA  ALA B 249     18.598  96.069  43.059  1.00 17.68      B   C
ATOM  3911 CB  ALA B 249     18.435  96.240  44.557  1.00 14.89      B   C
ATOM  3912 C   ALA B 249     19.210  97.332  42.449  1.00 16.19      B   C
ATOM  3913 O   ALA B 249     18.509  98.166  41.878  1.00 15.71      B   O
ATOM  3914 N   LYS B 250     20.523  97.466  42.578  1.00 15.67      B   N
ATOM  3915 CA  LYS B 250     21.221  98.625  42.039  1.00 16.75      B   C
ATOM  3916 CB  LYS B 250     22.686  98.599  42.493  1.00 20.71      B   C
ATOM  3917 CG  LYS B 250     23.555  99.725  41.952  1.00 24.70      B   C
ATOM  3918 CD  LYS B 250     23.089 101.093  42.425  1.00 29.48      B   C
ATOM  3919 CE  LYS B 250     24.028 102.180  41.914  1.00 34.06      B   C
ATOM  3920 NZ  LYS B 250     23.548 103.549  42.249  1.00 35.09      B   N
ATOM  3921 C   LYS B 250     21.137  98.633  40.514  1.00 16.02      B   C
ATOM  3922 O   LYS B 250     20.910  99.672  39.899  1.00 16.61      B   O
ATOM  3923 N   GLU B 251     21.300  97.464  39.907  1.00 16.92      B   N
ATOM  3924 CA  GLU B 251     21.256  97.366  38.457  1.00 16.87      B   C
ATOM  3925 CB  GLU B 251     21.789  96.009  38.000  1.00 17.15      B   C
ATOM  3926 CG  GLU B 251     21.913  95.902  36.492  1.00 19.76      B   C
ATOM  3927 CD  GLU B 251     22.195  94.495  36.030  1.00 21.03      B   C
ATOM  3928 OE1 GLU B 251     22.812  93.728  36.796  1.00 21.54      B   O
ATOM  3929 OE2 GLU B 251     21.813  94.159  34.891  1.00 23.50      B   O
ATOM  3930 C   GLU B 251     19.864  97.561  37.868  1.00 18.30      B   C
ATOM  3931 O   GLU B 251     19.696  98.297  36.895  1.00 18.23      B   O
ATOM  3932 N   TRP B 252     18.865  96.918  38.464  1.00 17.41      B   N
ATOM  3933 CA  TRP B 252     17.509  96.997  37.939  1.00 17.31      B   C
ATOM  3934 CB  TRP B 252     16.868  95.610  37.973  1.00 16.21      B   C
ATOM  3935 CG  TRP B 252     17.639  94.610  37.197  1.00 16.40      B   C
ATOM  3936 CD2 TRP B 252     17.650  94.459  35.775  1.00 17.43      B   C
ATOM  3937 CE2 TRP B 252     18.546  93.412  35.475  1.00 17.08      B   C
ATOM  3938 CE3 TRP B 252     16.988  95.107  34.723  1.00 20.12      B   C
ATOM  3939 CD1 TRP B 252     18.505  93.677  37.690  1.00 18.25      B   C
ATOM  3940 NE1 TRP B 252     19.053  92.954  36.662  1.00 17.57      B   N
ATOM  3941 CZ2 TRP B 252     18.799  92.996  34.167  1.00 16.27      B   C
ATOM  3942 CZ3 TRP B 252     17.239  94.691  33.416  1.00 18.36      B   C
ATOM  3943 CH2 TRP B 252     18.137  93.646  33.153  1.00 18.85      B   C
ATOM  3944 C   TRP B 252     16.555  98.000  38.565  1.00 20.68      B   C
ATOM  3945 O   TRP B 252     15.631  98.468  37.896  1.00 23.26      B   O
ATOM  3946 N   LEU B 253     16.762  98.333  39.833  1.00 20.19      B   N
ATOM  3947 CA  LEU B 253     15.878  99.279  40.508  1.00 22.15      B   C
ATOM  3948 CB  LEU B 253     15.392  98.680  41.832  1.00 19.99      B   C
ATOM  3949 CG  LEU B 253     14.796  97.269  41.748  1.00 20.08      B   C
ATOM  3950 CD1 LEU B 253     14.520  96.731  43.149  1.00 15.94      B   C
ATOM  3951 CD2 LEU B 253     13.521  97.299  40.918  1.00 20.16      B   C
ATOM  3952 C   LEU B 253     16.588 100.602  40.766  1.00 25.98      B   C
ATOM  3953 O   LEU B 253     15.971 101.573  41.213  1.00 28.88      B   O
ATOM  3954 N   LYS B 254     17.887 100.631  40.478  1.00 28.33      B   N
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Figure 7RRR

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ATOM  3955  CA  LYS B 254     18.713 101.822  40.684  1.00 32.00      B   C
ATOM  3956  CB  LYS B 254     18.210 102.985  39.818  1.00 33.97      B   C
ATOM  3957  CG  LYS B 254     17.844 102.597  38.388  1.00 37.77      B   C
ATOM  3958  CD  LYS B 254     18.983 101.890  37.661  1.00 38.80      B   C
ATOM  3959  CE  LYS B 254     18.544 101.453  36.265  1.00 41.63      B   C
ATOM  3960  NZ  LYS B 254     19.608 100.705  35.535  1.00 41.49      B   N
ATOM  3961  C   LYS B 254     18.677 102.214  42.162  1.00 32.29      B   C
ATOM  3962  O   LYS B 254     18.716 103.399  42.511  1.00 32.23      B   O
ATOM  3963  N   LEU B 255     18.603 101.201  43.022  1.00 31.24      B   N
ATOM  3964  CA  LEU B 255     18.560 101.397  44.469  1.00 34.52      B   C
ATOM  3965  CB  LEU B 255     17.250 100.844  45.039  1.00 34.04      B   C
ATOM  3966  CG  LEU B 255     15.917 101.437  44.584  1.00 36.59      B   C
ATOM  3967  CD1 LEU B 255     14.795 100.596  45.162  1.00 35.66      B   C
ATOM  3968  CD2 LEU B 255     15.791 102.888  45.036  1.00 36.85      B   C
ATOM  3969  C   LEU B 255     19.727 100.667  45.132  1.00 35.40      B   C
ATOM  3970  O   LEU B 255     20.326  99.794  44.473  1.00 34.56      B   O
ATOM  3971  OXT LEU B 255     20.014 100.959  46.310  1.00 38.02      B   O
ATOM  3992  C2  INH E   1     13.974  93.547  34.196  1.00 21.79      E   C
ATOM  3993  O11 INH E   1     13.261  94.464  33.777  1.00 21.09      E   O
ATOM  3994  N3  INH E   1     14.165  93.379  35.564  1.00 20.44      E   N
ATOM  3995  C7  INH E   1     13.557  94.278  36.569  1.00 20.49      E   C
ATOM  3996  C8  INH E   1     12.019  94.237  36.759  1.00 24.92      E   C
ATOM  3997  C10 INH E   1     11.708  94.941  38.091  1.00 25.12      E   C
ATOM  3998  C9  INH E   1     11.452  92.810  36.842  1.00 26.68      E   C
ATOM  3999  C4  INH E   1     14.957  92.363  36.018  1.00 19.38      E   C
ATOM  4000  N16 INH E   1     15.217  92.064  37.221  1.00 20.22      E   N
ATOM  4001  N15 INH E   1     16.020  90.988  37.236  1.00 18.99      E   N
ATOM  4002  C23 INH E   1     16.484  90.354  38.489  1.00 18.33      E   C
ATOM  4003  C24 INH E   1     15.792  88.946  38.541  1.00 19.18      E   C
ATOM  4004  C29 INH E   1     14.344  88.784  38.535  1.00 19.84      E   C
ATOM  4005  C30 INH E   1     13.446  89.896  38.512  1.00 20.83      E   C
ATOM  4006  C31 INH E   1     12.035  89.694  38.503  1.00 22.55      E   C
ATOM  4007  C32 INH E   1     11.503  88.377  38.513  1.00 24.46      E   C
ATOM  4008  C33 INH E   1     12.376  87.256  38.536  1.00 23.50      E   C
ATOM  4009  C28 INH E   1     13.783  87.448  38.549  1.00 21.97      E   C
ATOM  4010  C27 INH E   1     14.636  86.315  38.572  1.00 21.05      E   C
ATOM  4011  C26 INH E   1     16.045  86.483  38.584  1.00 19.47      E   C
ATOM  4012  C25 INH E   1     16.617  87.782  38.567  1.00 22.25      E   C
ATOM  4013  C14 INH E   1     16.294  90.592  35.978  1.00 15.83      E   C
ATOM  4014  C17 INH E   1     17.178  89.405  35.585  1.00 16.67      E   C
ATOM  4015  C22 INH E   1     18.577  89.438  35.898  1.00 19.23      E   C
ATOM  4016  C21 INH E   1     19.395  88.340  35.554  1.00 18.31      E   C
ATOM  4017  N20 INH E   1     18.850  87.251  34.923  1.00 19.45      E   N
ATOM  4018  C19 INH E   1     17.516  87.188  34.607  1.00 18.95      E   C
ATOM  4019  C18 INH E   1     16.650  88.261  34.930  1.00 20.05      E   C
ATOM  4020  C5  INH E   1     15.629  91.408  35.147  1.00 16.08      E   C
ATOM  4021  C6  INH E   1     15.419  91.604  33.697  1.00 18.68      E   C
ATOM  4022  O13 INH E   1     15.959  90.832  32.910  1.00 18.22      E   O
ATOM  4023  N1  INH E   1     14.594  92.661  33.309  1.00 20.12      E   N
ATOM  4024  C12 INH E   1     14.373  92.853  31.870  1.00 19.38      E   C
ATOM  4025  C2  INH F   1     15.229  56.504  36.336  1.00 19.66      F   C
ATOM  4026  O11 INH F   1     15.872  55.553  35.883  1.00 19.27      F   O
ATOM  4027  N3  INH F   1     15.347  56.832  37.680  1.00 18.37      F   N
ATOM  4028  C7  INH F   1     16.244  56.066  38.574  1.00 21.01      F   C
ATOM  4029  C8  INH F   1     17.632  56.714  38.844  1.00 22.14      F   C
ATOM  4030  C10 INH F   1     18.576  56.443  37.657  1.00 27.02      F   C
ATOM  4031  C9  INH F   1     18.283  56.135  40.116  1.00 26.97      F   C
ATOM  4032  C4  INH F   1     14.636  57.891  38.181  1.00 20.15      F   C
```

Figure 7SSS

```
ATOM  4033 N16 INH F   1      14.628  58.344  39.361  1.00 18.70      F   N
ATOM  4034 N15 INH F   1      13.787  59.404  39.418  1.00 20.10      F   N
ATOM  4035 C23 INH F   1      13.574  60.201  40.652  1.00 16.99      F   C
ATOM  4036 C24 INH F   1      14.177  61.615  40.365  1.00 16.25      F   C
ATOM  4037 C29 INH F   1      15.574  61.787  40.020  1.00 16.89      F   C
ATOM  4038 C30 INH F   1      16.491  60.678  39.950  1.00 17.51      F   C
ATOM  4039 C31 INH F   1      17.854  60.879  39.603  1.00 14.32      F   C
ATOM  4040 C32 INH F   1      18.324  62.192  39.315  1.00 19.70      F   C
ATOM  4041 C33 INH F   1      17.437  63.304  39.377  1.00 18.92      F   C
ATOM  4042 C28 INH F   1      16.071  63.112  39.727  1.00 19.84      F   C
ATOM  4043 C27 INH F   1      15.198  64.232  39.783  1.00 19.07      F   C
ATOM  4044 C26 INH F   1      13.829  64.056  40.129  1.00 19.02      F   C
ATOM  4045 C25 INH F   1      13.322  62.761  40.417  1.00 19.18      F   C
ATOM  4046 C14 INH F   1      13.224  59.615  38.219  1.00 20.53      F   C
ATOM  4047 C17 INH F   1      12.214  60.722  37.880  1.00 21.41      F   C
ATOM  4048 C22 INH F   1      10.902  60.683  38.443  1.00 24.07      F   C
ATOM  4049 C21 INH F   1       9.981  61.718  38.139  1.00 24.54      F   C
ATOM  4050 N20 INH F   1      10.356  62.748  37.310  1.00 24.94      F   N
ATOM  4051 C19 INH F   1      11.609  62.812  36.753  1.00 22.24      F   C
ATOM  4052 C18 INH F   1      12.564  61.805  37.024  1.00 22.59      F   C
ATOM  4053 C5  INH F   1      13.722  58.699  37.372  1.00 19.26      F   C
ATOM  4054 C6  INH F   1      13.620  58.311  35.947  1.00 19.59      F   C
ATOM  4055 O13 INH F   1      12.881  58.941  35.211  1.00 18.89      F   O
ATOM  4056 N1  INH F   1      14.371  57.239  35.521  1.00 18.86      F   N
ATOM  4057 C12 INH F   1      14.267  56.869  34.104  1.00 22.90      F   C
ATOM  4058 OH2 TIP S   1      26.694  70.185  39.535  1.00 10.43      S   O
ATOM  4059 OH2 TIP S   2      26.903  61.775  37.433  1.00 10.86      S   O
ATOM  4060 OH2 TIP S   3      35.118  64.928  45.661  1.00  9.77      S   O
ATOM  4061 OH2 TIP S   4       3.740  88.714  42.243  1.00 12.17      S   O
ATOM  4062 OH2 TIP S   5      -3.817  87.331  48.367  1.00 15.62      S   O
ATOM  4063 OH2 TIP S   6      16.515  80.411  54.861  1.00 15.64      S   O
ATOM  4064 OH2 TIP S   7      26.620  62.820  41.255  1.00 10.32      S   O
ATOM  4065 OH2 TIP S   8       3.173  81.112  41.277  1.00 12.87      S   O
ATOM  4066 OH2 TIP S   9      -5.009  77.145  39.859  1.00 14.54      S   O
ATOM  4067 OH2 TIP S  10      17.072  78.274  43.100  1.00 15.49      S   O
ATOM  4068 OH2 TIP S  11      11.094  82.014  54.953  1.00 13.66      S   O
ATOM  4069 OH2 TIP S  12      23.114  78.487  54.347  1.00 14.98      S   O
ATOM  4070 OH2 TIP S  13      20.046  86.513  47.218  1.00 13.55      S   O
ATOM  4071 OH2 TIP S  14       2.655  89.017  38.291  1.00 15.07      S   O
ATOM  4072 OH2 TIP S  15       9.228  70.350  55.121  1.00 12.46      S   O
ATOM  4073 OH2 TIP S  16      16.739  84.862  44.381  1.00 12.76      S   O
ATOM  4074 OH2 TIP S  17      25.567  61.078  39.581  1.00 14.41      S   O
ATOM  4075 OH2 TIP S  18      37.252  56.626  40.690  1.00 14.19      S   O
ATOM  4076 OH2 TIP S  19      18.275  89.911  32.191  1.00 17.34      S   O
ATOM  4077 OH2 TIP S  20      34.008  72.385  38.024  1.00 14.04      S   O
ATOM  4078 OH2 TIP S  21      -1.688  79.172  55.257  1.00 19.38      S   O
ATOM  4079 OH2 TIP S  22      22.366  80.667  29.821  1.00 24.75      S   O
ATOM  4080 OH2 TIP S  23      12.380  75.091  59.029  1.00 20.05      S   O
ATOM  4081 OH2 TIP S  24      22.730  75.591  37.990  1.00 18.05      S   O
ATOM  4082 OH2 TIP S  25      -4.035  89.431  50.414  1.00 17.74      S   O
ATOM  4083 OH2 TIP S  26       4.573  89.940  39.949  1.00 14.11      S   O
ATOM  4084 OH2 TIP S  27      -1.906  87.737  40.180  1.00 17.43      S   O
ATOM  4085 OH2 TIP S  28      10.589  69.698  44.737  1.00 21.71      S   O
ATOM  4086 OH2 TIP S  29      25.201  95.439  52.148  1.00 16.83      S   O
ATOM  4087 OH2 TIP S  30      -8.367  85.700  23.246  1.00 15.98      S   O
ATOM  4088 OH2 TIP S  31      35.982  63.130  47.769  1.00 15.06      S   O
ATOM  4089 OH2 TIP S  32      21.296  70.481  54.804  1.00 19.30      S   O
ATOM  4090 OH2 TIP S  33      20.570  73.504  39.900  1.00 18.13      S   O
```

Figure 7TTT

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ATOM  4091 OH2 TIP S  34      27.666  49.772  40.587  1.00 14.52      S   O
ATOM  4092 OH2 TIP S  35       9.700  74.285  55.955  1.00 16.17      S   O
ATOM  4093 OH2 TIP S  36      12.186  64.800  48.529  1.00 17.60      S   O
ATOM  4094 OH2 TIP S  37      13.322  82.831  56.421  1.00 13.15      S   O
ATOM  4095 OH2 TIP S  38      34.693  38.751  49.392  1.00 20.67      S   O
ATOM  4096 OH2 TIP S  39      -5.001  91.649  54.454  1.00 20.34      S   O
ATOM  4097 OH2 TIP S  40      15.761  67.824  58.496  1.00 21.39      S   O
ATOM  4098 OH2 TIP S  41      11.148  84.424  43.877  1.00 12.67      S   O
ATOM  4099 OH2 TIP S  42      37.642  61.003  46.856  1.00 17.93      S   O
ATOM  4100 OH2 TIP S  43      -4.373  79.173  41.785  1.00 16.71      S   O
ATOM  4101 OH2 TIP S  44      43.723  52.077  51.584  1.00 18.94      S   O
ATOM  4102 OH2 TIP S  45      20.137  97.010  51.207  1.00 22.61      S   O
ATOM  4103 OH2 TIP S  46      -4.186  94.391  33.354  1.00 24.48      S   O
ATOM  4104 OH2 TIP S  47      10.434  59.744  34.860  1.00 20.09      S   O
ATOM  4105 OH2 TIP S  48      11.296  69.306  47.243  1.00 20.43      S   O
ATOM  4106 OH2 TIP S  49      13.514  84.678  43.033  1.00 17.25      S   O
ATOM  4107 OH2 TIP S  50      27.738  70.677  61.698  1.00 22.46      S   O
ATOM  4108 OH2 TIP S  51      16.289  72.356  55.129  1.00 13.74      S   O
ATOM  4109 OH2 TIP S  52      -4.477  95.904  37.489  1.00 27.31      S   O
ATOM  4110 OH2 TIP S  53      34.164  74.207  35.803  1.00 16.19      S   O
ATOM  4111 OH2 TIP S  54      13.181  73.070  43.734  1.00 17.17      S   O
ATOM  4112 OH2 TIP S  55      -3.958  90.260  57.512  1.00 25.11      S   O
ATOM  4113 OH2 TIP S  56      30.703  42.485  54.038  1.00 21.11      S   O
ATOM  4114 OH2 TIP S  57      30.922  56.349  27.885  1.00 20.13      S   O
ATOM  4115 OH2 TIP S  58      14.662  74.601  55.720  1.00 22.72      S   O
ATOM  4116 OH2 TIP S  59      38.507  59.138  50.812  1.00 19.14      S   O
ATOM  4117 OH2 TIP S  60      42.816  67.475  28.609  1.00 20.79      S   O
ATOM  4118 OH2 TIP S  61      -6.400  95.465  43.206  1.00 18.25      S   O
ATOM  4119 OH2 TIP S  62       6.561 102.864  47.606  1.00 21.89      S   O
ATOM  4120 OH2 TIP S  63      35.560  76.427  29.271  1.00 20.86      S   O
ATOM  4121 OH2 TIP S  64       5.810  69.019  32.123  1.00 25.31      S   O
ATOM  4122 OH2 TIP S  65      30.127  54.457  33.804  1.00 22.20      S   O
ATOM  4123 OH2 TIP S  66      14.517  98.509  59.915  1.00 20.97      S   O
ATOM  4124 OH2 TIP S  67      20.921  81.728  55.488  1.00 15.12      S   O
ATOM  4125 OH2 TIP S  68      18.125  78.127  55.061  1.00 22.38      S   O
ATOM  4126 OH2 TIP S  69       4.578 106.224  53.414  1.00 23.88      S   O
ATOM  4127 OH2 TIP S  70     -13.259  95.151  42.403  1.00 22.02      S   O
ATOM  4128 OH2 TIP S  71      19.506  66.848  43.948  1.00 14.64      S   O
ATOM  4129 OH2 TIP S  72      20.492  58.168  29.357  1.00 24.23      S   O
ATOM  4130 OH2 TIP S  73      14.362  66.682  45.311  1.00 21.95      S   O
ATOM  4131 OH2 TIP S  74      37.948  64.500  49.199  1.00 22.89      S   O
ATOM  4132 OH2 TIP S  75      22.382  83.107  46.881  1.00 21.36      S   O
ATOM  4133 OH2 TIP S  76       2.257  71.707  33.743  1.00 22.26      S   O
ATOM  4134 OH2 TIP S  77      28.562  50.607  60.811  1.00 23.59      S   O
ATOM  4135 OH2 TIP S  78      12.908  55.269  54.605  1.00 22.04      S   O
ATOM  4136 OH2 TIP S  79      23.712  82.581  52.850  1.00 18.46      S   O
ATOM  4137 OH2 TIP S  80       6.000  64.702  50.376  1.00 22.24      S   O
ATOM  4138 OH2 TIP S  81      31.597  63.665  38.013  1.00 16.06      S   O
ATOM  4139 OH2 TIP S  82       3.204 101.393  39.851  1.00 18.09      S   O
ATOM  4140 OH2 TIP S  83      -3.695  88.746  62.013  1.00 24.84      S   O
ATOM  4141 OH2 TIP S  84      17.546  65.110  21.326  1.00 19.55      S   O
ATOM  4142 OH2 TIP S  85      26.824  59.347  62.759  1.00 26.30      S   O
ATOM  4143 OH2 TIP S  86      29.013  78.700  36.194  1.00 29.19      S   O
ATOM  4144 OH2 TIP S  87     -21.912  84.760  37.477  1.00 26.29      S   O
ATOM  4145 OH2 TIP S  88      37.659  49.564  54.905  1.00 21.54      S   O
ATOM  4146 OH2 TIP S  89      15.623  89.654  61.494  1.00 20.60      S   O
ATOM  4147 OH2 TIP S  90      46.913  73.636  27.864  1.00 24.09      S   O
ATOM  4148 OH2 TIP S  91      31.635  68.716  13.795  1.00 26.68      S   O
```

Figure 7UUU

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ATOM  4149 OH2 TIP S  92      8.998  77.444  41.106  1.00 21.52      S   O
ATOM  4150 OH2 TIP S  93     19.563  69.848  56.803  1.00 23.78      S   O
ATOM  4151 OH2 TIP S  94     21.054  77.796  57.903  1.00 20.91      S   O
ATOM  4152 OH2 TIP S  95     39.029  70.195  42.752  1.00 19.43      S   O
ATOM  4153 OH2 TIP S  96     16.357  59.879  28.472  1.00 34.72      S   O
ATOM  4154 OH2 TIP S  97      6.277  85.600  21.656  1.00 18.30      S   O
ATOM  4155 OH2 TIP S  98     24.381  79.010  25.797  1.00 24.45      S   O
ATOM  4156 OH2 TIP S  99     -0.330  73.515  46.326  1.00 21.44      S   O
ATOM  4157 OH2 TIP S 100     19.996  63.469  21.479  1.00 20.07      S   O
ATOM  4158 OH2 TIP S 101      8.484  64.804  37.057  1.00 21.03      S   O
ATOM  4159 OH2 TIP S 102     18.063  76.067  36.689  1.00 20.99      S   O
ATOM  4160 OH2 TIP S 103     13.804  68.104  43.044  1.00 25.16      S   O
ATOM  4161 OH2 TIP S 104     10.019  70.355  50.629  1.00 23.39      S   O
ATOM  4162 OH2 TIP S 105     36.764  63.450  55.390  1.00 19.23      S   O
ATOM  4163 OH2 TIP S 106     -3.017  81.106  52.043  1.00 29.08      S   O
ATOM  4164 OH2 TIP S 107     33.894  73.874  51.602  1.00 22.56      S   O
ATOM  4165 OH2 TIP S 108    -10.562  79.620  30.884  1.00 25.06      S   O
ATOM  4166 OH2 TIP S 109     -3.241  87.887  16.187  1.00 22.20      S   O
ATOM  4167 OH2 TIP S 110     36.320  79.997  40.961  1.00 30.47      S   O
ATOM  4168 OH2 TIP S 111     12.536  71.003  57.233  1.00 20.62      S   O
ATOM  4169 OH2 TIP S 112     -0.943  95.950  34.554  1.00 25.68      S   O
ATOM  4170 OH2 TIP S 113     14.938  45.779  46.539  1.00 32.69      S   O
ATOM  4171 OH2 TIP S 114     44.541  72.750  24.779  1.00 28.57      S   O
ATOM  4172 OH2 TIP S 115     16.028  56.338  61.884  1.00 27.69      S   O
ATOM  4173 OH2 TIP S 116     25.959  84.862  44.510  1.00 22.27      S   O
ATOM  4174 OH2 TIP S 117     11.898  70.641  40.303  1.00 29.38      S   O
ATOM  4175 OH2 TIP S 118     20.005  82.352  45.778  1.00 23.69      S   O
ATOM  4176 OH2 TIP S 119     24.653  82.113  42.509  1.00 26.73      S   O
ATOM  4177 OH2 TIP S 120     39.045  70.244  55.129  1.00 26.86      S   O
ATOM  4178 OH2 TIP S 121    -14.861  94.263  30.815  1.00 25.70      S   O
ATOM  4179 OH2 TIP S 122     28.805  79.348  55.384  1.00 24.42      S   O
ATOM  4180 OH2 TIP S 123     34.409  78.819  35.704  1.00 22.51      S   O
ATOM  4181 OH2 TIP S 124     25.708  95.887  48.431  1.00 22.52      S   O
ATOM  4182 OH2 TIP S 125     20.200  81.715  43.235  1.00 28.28      S   O
ATOM  4183 OH2 TIP S 126      8.358  89.545  27.306  1.00 25.44      S   O
ATOM  4184 OH2 TIP S 127     28.451  42.142  55.370  1.00 32.71      S   O
ATOM  4185 OH2 TIP S 128     -1.140  72.535  35.377  1.00 25.03      S   O
ATOM  4186 OH2 TIP S 129     42.723  73.261  29.197  1.00 26.01      S   O
ATOM  4187 OH2 TIP S 130      0.475 106.754  43.565  1.00 35.60      S   O
ATOM  4188 OH2 TIP S 131     -8.799  81.517  47.238  1.00 30.82      S   O
ATOM  4189 OH2 TIP S 132     18.817  63.647  62.682  1.00 23.39      S   O
ATOM  4190 OH2 TIP S 133    -14.788  83.367  33.703  1.00 22.25      S   O
ATOM  4191 OH2 TIP S 134     28.486  47.289  40.587  1.00 26.04      S   O
ATOM  4192 OH2 TIP S 135     13.709  66.288  58.292  1.00 31.84      S   O
ATOM  4193 OH2 TIP S 136      4.869  72.011  43.934  1.00 21.85      S   O
ATOM  4194 OH2 TIP S 137    -19.103  77.442  35.205  1.00 29.80      S   O
ATOM  4195 OH2 TIP S 138     20.407  79.490  35.831  1.00 35.16      S   O
ATOM  4196 OH2 TIP S 139     10.860  84.010  22.443  1.00 27.02      S   O
ATOM  4197 OH2 TIP S 140      0.151 101.506  60.922  1.00 25.88      S   O
ATOM  4198 OH2 TIP S 141     31.584  47.279  41.254  1.00 23.80      S   O
ATOM  4199 OH2 TIP S 142     38.066  70.701  25.990  1.00 19.24      S   O
ATOM  4200 OH2 TIP S 143     44.977  72.631  31.204  1.00 23.78      S   O
ATOM  4201 OH2 TIP S 144     10.719  65.231  40.054  1.00 26.38      S   O
ATOM  4202 OH2 TIP S 145      7.475  91.297  29.034  1.00 27.02      S   O
ATOM  4203 OH2 TIP S 146     37.874  61.748  52.268  1.00 29.73      S   O
ATOM  4204 OH2 TIP S 147     -5.574  93.894  53.509  1.00 23.66      S   O
ATOM  4205 OH2 TIP S 148     17.820  78.905  36.654  1.00 28.79      S   O
ATOM  4206 OH2 TIP S 149     29.549  83.050  48.881  1.00 26.52      S   O
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Figure 7VVV

```
ATOM  4207  OH2 TIP S 150   -10.366 100.932  54.067  1.00 20.68      S   O
ATOM  4208  OH2 TIP S 151    30.504  64.646  60.794  1.00 28.37      S   O
ATOM  4209  OH2 TIP S 152    49.012  70.756  24.772  1.00 31.55      S   O
ATOM  4210  OH2 TIP S 153    30.846  45.257  57.188  1.00 31.72      S   O
ATOM  4211  OH2 TIP S 154    43.180  59.055  25.923  1.00 26.29      S   O
ATOM  4212  OH2 TIP S 155    22.523  66.585  65.647  1.00 32.96      S   O
ATOM  4213  OH2 TIP S 156     2.253 106.632  56.997  1.00 37.06      S   O
ATOM  4214  OH2 TIP S 157    21.987  90.927  36.214  1.00 24.25      S   O
ATOM  4215  OH2 TIP S 158    24.995  45.779  50.248  1.00 28.19      S   O
ATOM  4216  OH2 TIP S 159    24.701  87.274  52.417  1.00 25.41      S   O
ATOM  4217  OH2 TIP S 160    19.481  54.793  61.669  1.00 24.28      S   O
ATOM  4218  OH2 TIP S 161     5.052  66.267  52.559  1.00 20.50      S   O
ATOM  4219  OH2 TIP S 162    24.083  47.425  48.238  1.00 32.20      S   O
ATOM  4220  OH2 TIP S 163    50.567  67.161  31.028  1.00 21.83      S   O
ATOM  4221  OH2 TIP S 164    15.358  64.805  23.213  1.00 24.49      S   O
ATOM  4222  OH2 TIP S 165    -1.913  91.256  42.961  1.00 21.23      S   O
ATOM  4223  OH2 TIP S 166    32.576  60.552  40.991  1.00 24.61      S   O
ATOM  4224  OH2 TIP S 167     5.829  70.768  57.525  1.00 22.41      S   O
ATOM  4225  OH2 TIP S 168     6.357  83.074  62.946  1.00 20.77      S   O
ATOM  4226  OH2 TIP S 169    28.962  85.053  47.200  1.00 36.42      S   O
ATOM  4227  OH2 TIP S 170    22.828  55.785  37.965  1.00 34.04      S   O
ATOM  4228  OH2 TIP S 171     9.903 109.166  51.388  1.00 29.79      S   O
ATOM  4229  OH2 TIP S 172     6.629  71.093  33.592  1.00 24.39      S   O
ATOM  4230  OH2 TIP S 173    24.428  80.747  55.009  1.00 17.22      S   O
ATOM  4231  OH2 TIP S 174    11.049  67.896  25.243  1.00 28.73      S   O
ATOM  4232  OH2 TIP S 175    26.525  84.672  50.346  1.00 22.59      S   O
ATOM  4233  OH2 TIP S 176    14.485  79.387  59.276  1.00 36.33      S   O
ATOM  4234  OH2 TIP S 178    -8.133  88.350  22.930  1.00 24.98      S   O
ATOM  4235  OH2 TIP S 179    11.008  89.282  26.933  1.00 26.38      S   O
ATOM  4236  OH2 TIP S 180    29.198  77.232  57.047  1.00 28.34      S   O
ATOM  4237  OH2 TIP S 181    42.985  63.495  21.723  1.00 32.93      S   O
ATOM  4238  OH2 TIP S 182    -2.488  92.239  26.844  1.00 31.41      S   O
ATOM  4239  OH2 TIP S 183    38.070  68.391  49.950  1.00 27.44      S   O
ATOM  4240  OH2 TIP S 184     3.026  87.382  17.697  1.00 24.17      S   O
ATOM  4241  OH2 TIP S 185    32.032  45.265  50.288  1.00 26.40      S   O
ATOM  4242  OH2 TIP S 186    39.904  55.447  42.177  1.00 25.49      S   O
ATOM  4243  OH2 TIP S 187     2.867  70.555  28.600  1.00 25.55      S   O
ATOM  4244  OH2 TIP S 188    28.784  77.898  31.205  1.00 27.78      S   O
ATOM  4245  OH2 TIP S 189     6.525  74.751  39.761  1.00 27.53      S   O
ATOM  4246  OH2 TIP S 190    -6.708  81.142  14.878  1.00 30.15      S   O
ATOM  4247  OH2 TIP S 191    23.949  87.249  38.410  1.00 26.94      S   O
ATOM  4248  OH2 TIP S 192     5.279  83.214  19.647  1.00 23.04      S   O
ATOM  4249  OH2 TIP S 193     7.787  93.915  65.832  1.00 34.56      S   O
ATOM  4250  OH2 TIP S 194    40.056  62.665  49.571  1.00 45.56      S   O
ATOM  4251  OH2 TIP S 195    17.005  83.158  42.309  1.00 26.09      S   O
ATOM  4252  OH2 TIP S 196    39.783  52.482  36.066  1.00 43.89      S   O
ATOM  4253  OH2 TIP S 197    21.034  85.408  34.631  1.00 21.18      S   O
ATOM  4254  OH2 TIP S 198    -2.760  93.994  35.518  1.00 32.71      S   O
ATOM  4255  OH2 TIP S 199   -14.876  77.201  34.781  1.00 29.91      S   O
ATOM  4256  OH2 TIP S 200     7.796  94.208  62.630  1.00 34.21      S   O
ATOM  4257  OH2 TIP S 201   -10.407  94.563  54.451  1.00 30.66      S   O
ATOM  4258  OH2 TIP S 202    19.132  85.088  38.251  1.00 26.36      S   O
ATOM  4259  OH2 TIP S 203    46.329  71.427  42.245  1.00 38.45      S   O
ATOM  4260  OH2 TIP S 204    38.151  49.728  42.054  1.00 23.90      S   O
ATOM  4261  OH2 TIP S 205   -16.881  92.357  37.722  1.00 29.19      S   O
ATOM  4262  OH2 TIP S 206     8.018  58.831  39.198  1.00 17.50      S   O
ATOM  4263  OH2 TIP S 207    23.689  77.990  32.612  1.00 37.51      S   O
ATOM  4264  OH2 TIP S 208    30.303  45.065  54.676  1.00 28.16      S   O
```

Figure 7WWW

```
ATOM  4265  OH2 TIP S 209      25.161  84.823  52.568  1.00 29.69      S   O
ATOM  4266  OH2 TIP S 210      23.062  78.703  21.684  1.00 26.51      S   O
ATOM  4267  OH2 TIP S 211      26.355  47.512  59.226  1.00 41.38      S   O
ATOM  4268  OH2 TIP S 212      12.364  73.834  56.670  1.00 17.58      S   O
ATOM  4269  OH2 TIP S 213      22.789 101.251  38.634  1.00 36.48      S   O
ATOM  4270  OH2 TIP S 214      30.444  78.274  42.812  1.00 18.27      S   O
ATOM  4271  OH2 TIP S 215      16.714  66.636  43.404  1.00 27.82      S   O
ATOM  4272  OH2 TIP S 216      11.118 110.647  48.883  1.00 41.21      S   O
ATOM  4273  OH2 TIP S 217      11.938  77.223  62.477  1.00 26.78      S   O
ATOM  4274  OH2 TIP S 218      21.348  98.318  46.299  1.00 22.54      S   O
ATOM  4275  OH2 TIP S 219       6.335  90.109  61.055  1.00 30.93      S   O
ATOM  4276  OH2 TIP S 220      16.849  58.092  31.635  1.00 27.78      S   O
ATOM  4277  OH2 TIP S 221     -14.977  98.435  36.110  1.00 29.94      S   O
ATOM  4278  OH2 TIP S 222      32.209  56.644  34.417  1.00 27.61      S   O
ATOM  4279  OH2 TIP S 223      38.616  69.338  19.683  1.00 35.00      S   O
ATOM  4280  OH2 TIP S 224      43.793  66.187  40.980  1.00 28.57      S   O
ATOM  4281  OH2 TIP S 225      25.865  49.291  48.912  1.00 22.19      S   O
ATOM  4282  OH2 TIP S 226      29.493  51.282  39.294  1.00 28.59      S   O
ATOM  4283  OH2 TIP S 227       8.557  68.734  23.715  1.00 32.38      S   O
ATOM  4284  OH2 TIP S 228      35.030  72.215  49.061  1.00 21.47      S   O
ATOM  4285  OH2 TIP S 229      -5.863  84.407  53.693  1.00 32.71      S   O
ATOM  4286  OH2 TIP S 230       8.409  66.822  21.454  1.00 32.17      S   O
ATOM  4287  OH2 TIP S 231      16.090  88.535  25.766  1.00 45.41      S   O
ATOM  4288  OH2 TIP S 232       5.228  66.001  48.372  1.00 33.03      S   O
ATOM  4289  OH2 TIP S 233      22.372  81.334  39.929  1.00 38.56      S   O
ATOM  4290  OH2 TIP S 234     -11.344  82.468  23.312  1.00 32.37      S   O
ATOM  4291  OH2 TIP S 235      -5.663  88.297  52.367  1.00 28.46      S   O
ATOM  4292  OH2 TIP S 236      13.616  74.457  18.786  1.00 42.18      S   O
ATOM  4293  OH2 TIP S 237      25.283  53.133  37.923  1.00 40.56      S   O
ATOM  4294  OH2 TIP S 238       8.026  53.624  54.137  1.00 31.65      S   O
ATOM  4295  OH2 TIP S 239      34.534  62.367  11.800  1.00 31.60      S   O
ATOM  4296  OH2 TIP S 240       1.831  56.099  44.184  1.00 34.48      S   O
ATOM  4297  OH2 TIP S 241      49.497  62.599  26.810  1.00 26.78      S   O
ATOM  4298  OH2 TIP S 242      -4.758  72.368  21.533  1.00 38.11      S   O
ATOM  4299  OH2 TIP S 243      -5.868  83.431  58.623  1.00 34.40      S   O
ATOM  4300  OH2 TIP S 244      29.156  81.797  37.170  1.00 39.60      S   O
ATOM  4301  OH2 TIP S 245      21.609  85.611  37.638  1.00 20.34      S   O
ATOM  4302  OH2 TIP S 246      -4.284  77.490  49.709  1.00 35.30      S   O
ATOM  4303  OH2 TIP S 247      31.807  48.664  61.432  1.00 43.66      S   O
ATOM  4304  OH2 TIP S 248      34.652  80.273  32.759  1.00 35.30      S   O
ATOM  4305  OH2 TIP S 249      -7.767  74.088  33.904  1.00 27.76      S   O
ATOM  4306  OH2 TIP S 250      -0.973  76.943  21.093  1.00 36.81      S   O
ATOM  4307  OH2 TIP S 251      17.520 103.841  50.759  1.00 37.13      S   O
ATOM  4308  OH2 TIP S 252      36.677  59.162  23.943  1.00 39.63      S   O
ATOM  4309  OH2 TIP S 253      -3.985  93.307  65.493  1.00 38.58      S   O
ATOM  4310  OH2 TIP S 254      26.053  53.836  34.851  1.00 37.31      S   O
ATOM  4311  OH2 TIP S 255      -7.010  78.156  28.377  1.00 28.40      S   O
ATOM  4312  OH2 TIP S 256       3.198  69.864  24.836  1.00 24.87      S   O
ATOM  4313  OH2 TIP S 257      -2.729  89.793  59.984  1.00 35.90      S   O
ATOM  4314  OH2 TIP S 259      12.874  62.780  21.486  1.00 40.71      S   O
ATOM  4315  OH2 TIP S 260      34.460  53.900  62.259  1.00 37.85      S   O
ATOM  4316  OH2 TIP S 261       8.524  50.114  40.677  1.00 29.93      S   O
ATOM  4317  OH2 TIP S 262      13.534  51.901  52.802  1.00 35.55      S   O
ATOM  4318  OH2 TIP S 263      -5.651  71.332  27.984  1.00 36.22      S   O
ATOM  4319  OH2 TIP S 264      10.884  74.117  37.648  1.00 23.87      S   O
ATOM  4320  OH2 TIP S 265       1.558 105.085  59.290  1.00 30.99      S   O
ATOM  4321  OH2 TIP S 267      22.855  87.241  54.244  1.00 39.85      S   O
ATOM  4322  OH2 TIP S 268      19.606  84.810  44.816  1.00 16.00      S   O
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Figure 7XXX

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ATOM  4323  OH2 TIP S 269     10.246  57.810  32.854  1.00 25.86      S   O
ATOM  4324  OH2 TIP S 270    -21.599  79.618  39.328  1.00 38.76      S   O
ATOM  4325  OH2 TIP S 271     35.642  69.502  46.091  1.00 25.61      S   O
ATOM  4326  OH2 TIP S 272      7.124  71.606  39.935  1.00 32.52      S   O
ATOM  4327  OH2 TIP S 274     37.219  53.704  29.589  1.00 30.49      S   O
ATOM  4328  OH2 TIP S 275     15.688  71.656  41.660  1.00 35.47      S   O
ATOM  4329  OH2 TIP S 276     18.771  98.089  33.479  1.00 36.76      S   O
ATOM  4330  OH2 TIP S 277     18.891  96.723  59.037  1.00 34.81      S   O
ATOM  4331  OH2 TIP S 279     20.582  96.155  32.990  1.00 36.72      S   O
ATOM  4332  OH2 TIP S 280     38.382  46.507  54.083  1.00 22.09      S   O
ATOM  4333  OH2 TIP S 284     33.499  78.469  29.422  1.00 42.54      S   O
ATOM  4334  OH2 TIP S 285     43.663  56.107  27.511  1.00 34.42      S   O
ATOM  4335  OH2 TIP S 286     35.122  60.670  20.712  1.00 39.38      S   O
ATOM  4336  OH2 TIP S 287     -1.725  96.233  63.363  1.00 35.97      S   O
ATOM  4337  OH2 TIP S 290     18.717  83.949  40.601  1.00 23.89      S   O
ATOM  4338  OH2 TIP S 291     38.772  45.987  46.680  1.00 36.15      S   O
ATOM  4339  OH2 TIP S 292     20.224  69.382  59.695  1.00 29.64      S   O
ATOM  4340  OH2 TIP S 293      8.282  78.199  63.669  1.00 36.59      S   O
ATOM  4341  OH2 TIP S 294     14.047  63.860  59.319  1.00 44.69      S   O
ATOM  4342  OH2 TIP S 297     -5.817  72.739  40.818  1.00 38.14      S   O
ATOM  4343  OH2 TIP S 298     26.321  64.439  12.786  1.00 45.15      S   O
ATOM  4344  OH2 TIP S 299     -6.944 102.099  43.661  1.00 28.91      S   O
ATOM  4345  OH2 TIP S 300     31.982  51.444  38.891  1.00 26.30      S   O
ATOM  4346  OH2 TIP S 301     22.179  61.349  17.217  1.00 28.54      S   O
ATOM  4347  OH2 TIP S 302     11.846  66.672  46.440  1.00 15.33      S   O
ATOM  4348  OH2 TIP S 303     16.579  61.209  61.822  1.00 25.84      S   O
ATOM  4349  OH2 TIP S 304      9.179  61.102  31.089  1.00 35.18      S   O
ATOM  4350  OH2 TIP S 306     43.337  56.983  38.631  1.00 31.17      S   O
ATOM  4351  OH2 TIP S 307     -4.729  79.060  14.954  1.00 29.45      S   O
ATOM  4352  OH2 TIP S 309      3.264  96.531  34.343  1.00 35.87      S   O
ATOM  4353  OH2 TIP S 310     33.597  56.115  32.020  1.00 38.28      S   O
ATOM  4354  OH2 TIP S 312     21.131  84.199  42.642  1.00 16.36      S   O
ATOM  4355  OH2 TIP S 314     13.289  90.298  22.035  1.00 37.86      S   O
ATOM  4356  OH2 TIP S 315    -21.318  88.597  32.650  1.00 31.68      S   O
ATOM  4357  OH2 TIP S 316      0.324  97.812  61.903  1.00 28.65      S   O
ATOM  4358  OH2 TIP S 317     15.681  48.773  53.561  1.00 32.11      S   O
ATOM  4359  OH2 TIP S 318      6.414  66.203  28.644  1.00 45.39      S   O
ATOM  4360  OH2 TIP S 320     21.877  45.789  57.051  1.00 37.88      S   O
ATOM  4361  OH2 TIP S 325     33.257  76.751  48.828  1.00 36.69      S   O
ATOM  4362  OH2 TIP S 326     -1.477  99.714  39.504  1.00 31.96      S   O
ATOM  4363  OH2 TIP S 327      7.083 107.442  40.232  1.00 34.50      S   O
ATOM  4364  OH2 TIP S 328     19.455  81.284  39.450  1.00 31.13      S   O
ATOM  4365  OH2 TIP S 330     18.928  59.678  27.698  1.00 23.64      S   O
ATOM  4366  OH2 TIP S 333      2.949  68.265  43.594  1.00 46.66      S   O
ATOM  4367  OH2 TIP S 334     -8.138 104.339  45.239  1.00 36.83      S   O
ATOM  4368  OH2 TIP S 336      3.891  58.458  48.159  1.00 40.09      S   O
ATOM  4369  OH2 TIP S 339    -11.491  79.098  22.692  1.00 31.58      S   O
ATOM  4370  OH2 TIP S 342     -3.605  77.350  56.479  1.00 33.40      S   O
ATOM  4371  OH2 TIP S 345     48.945  64.149  23.906  1.00 33.98      S   O
ATOM  4372  OH2 TIP S 348     17.597  50.879  59.000  1.00 46.70      S   O
ATOM  4373  OH2 TIP S 349    -19.548  99.216  33.850  1.00 31.30      S   O
ATOM  4374  OH2 TIP S 350     11.566  66.969  42.047  1.00 25.33      S   O
ATOM  4375  OH2 TIP S 353     24.674  43.379  42.738  1.00 46.49      S   O
ATOM  4376  OH2 TIP S 354     20.654  78.836  55.418  1.00 19.53      S   O
ATOM  4377  OH2 TIP S 357     17.254  91.782  60.031  1.00 23.92      S   O
ATOM  4378  OH2 TIP S 358      9.923  67.047  44.491  1.00 20.59      S   O
ATOM  4379  OH2 TIP S 359     36.952  66.998  45.661  1.00 21.28      S   O
ATOM  4380  OH2 TIP S 360     15.012  70.447  58.501  1.00 20.49      S   O
```

Figure 7YYY

ATOM 4381 OH2 TIP S 361 38.560 66.828 47.799 1.00 18.16 S O
ATOM 4382 OH2 TIP S 362 12.567 70.351 43.331 1.00 21.60 S O
ATOM 4383 OH2 TIP S 363 10.275 70.909 59.173 1.00 20.25 S O
ATOM 4384 OH2 TIP S 365 -8.636 80.604 29.420 1.00 20.84 S O
ATOM 4385 OH2 TIP S 366 27.535 82.312 43.508 1.00 25.30 S O
ATOM 4386 OH2 TIP S 367 17.257 86.397 26.338 1.00 29.08 S O
ATOM 4387 OH2 TIP S 368 4.358 55.280 44.796 1.00 40.14 S O
ATOM 4388 OH2 TIP S 369 8.463 83.561 21.334 1.00 22.41 S O
ATOM 4389 OH2 TIP S 370 -8.086 97.612 37.816 1.00 25.46 S O
ATOM 4390 OH2 TIP S 371 12.843 74.928 39.116 1.00 31.70 S O
ATOM 4391 OH2 TIP S 372 8.347 72.232 57.105 1.00 25.70 S O
ATOM 4392 OH2 TIP S 373 -3.834 109.911 52.412 1.00 25.46 S O
ATOM 4393 OH2 TIP S 374 38.734 67.042 43.751 1.00 25.21 S O
ATOM 4394 OH2 TIP S 375 20.952 90.132 33.041 1.00 26.25 S O
ATOM 4395 OH2 TIP S 376 21.122 98.404 49.083 1.00 21.33 S O
ATOM 4396 OH2 TIP S 377 -12.795 97.771 42.948 1.00 27.19 S O
ATOM 4397 OH2 TIP S 378 24.316 79.549 28.534 1.00 25.40 S O
ATOM 4398 OH2 TIP S 379 27.736 88.375 45.434 1.00 29.24 S O
ATOM 4399 OH2 TIP S 380 8.225 59.683 36.172 1.00 24.77 S O
ATOM 4400 OH2 TIP S 381 37.450 53.227 35.003 1.00 32.48 S O
ATOM 4401 OH2 TIP S 382 -10.586 84.900 22.199 1.00 30.47 S O
ATOM 4402 OH2 TIP S 383 -15.137 95.854 40.707 1.00 25.76 S O
ATOM 4403 OH2 TIP S 384 16.777 65.477 62.229 1.00 26.46 S O
ATOM 4404 OH2 TIP S 385 28.839 86.168 50.617 1.00 33.26 S O
ATOM 4405 OH2 TIP S 386 17.382 84.892 57.199 1.00 22.87 S O
ATOM 4406 OH2 TIP S 387 27.000 52.190 62.926 1.00 27.15 S O
ATOM 4407 OH2 TIP S 388 31.661 79.835 35.615 1.00 28.03 S O
ATOM 4408 OH2 TIP S 389 -4.676 84.758 48.894 1.00 31.68 S O
ATOM 4409 OH2 TIP S 390 -5.662 91.557 50.040 1.00 31.19 S O
ATOM 4410 OH2 TIP S 391 23.487 83.965 44.473 1.00 28.65 S O
ATOM 4411 OH2 TIP S 392 -6.441 88.875 58.175 1.00 33.33 S O
ATOM 4412 OH2 TIP S 393 7.603 93.526 36.250 1.00 30.57 S O
ATOM 4413 OH2 TIP S 394 49.203 72.825 26.301 1.00 24.46 S O
ATOM 4414 OH2 TIP S 395 28.479 61.371 62.617 1.00 32.12 S O
ATOM 4415 OH2 TIP S 397 -9.168 83.076 17.253 1.00 25.74 S O
ATOM 4416 OH2 TIP S 398 16.075 88.965 63.990 1.00 30.49 S O
ATOM 4417 OH2 TIP S 400 13.310 95.842 67.259 1.00 29.76 S O
ATOM 4418 OH2 TIP S 401 5.918 66.938 33.592 1.00 31.14 S O
ATOM 4419 OH2 TIP S 402 0.155 106.248 55.777 1.00 32.60 S O
ATOM 4420 OH2 TIP S 403 6.110 92.248 62.655 1.00 27.95 S O
ATOM 4421 OH2 TIP S 404 2.233 103.880 39.763 1.00 31.52 S O
ATOM 4422 OH2 TIP S 405 25.694 98.715 48.972 1.00 29.93 S O
ATOM 4423 OH2 TIP S 406 10.674 73.231 60.407 1.00 31.34 S O
ATOM 4424 OH2 TIP S 409 51.882 66.157 29.120 1.00 26.96 S O
ATOM 4425 OH2 TIP S 410 6.325 68.647 46.053 1.00 34.29 S O
ATOM 4426 OH2 TIP S 412 39.391 64.285 54.825 1.00 28.64 S O
ATOM 4427 OH2 TIP S 413 -2.620 73.079 47.858 1.00 31.55 S O
ATOM 4428 OH2 TIP S 414 32.879 78.973 43.464 1.00 29.58 S O
ATOM 4429 OH2 TIP S 415 -15.016 96.572 33.202 1.00 45.53 S O
ATOM 4430 OH2 TIP S 416 39.377 75.743 32.551 1.00 30.17 S O
ATOM 4431 OH2 TIP S 417 31.294 47.074 59.585 1.00 32.29 S O
ATOM 4432 OH2 TIP S 418 20.908 99.085 60.072 1.00 33.84 S O
ATOM 4433 OH2 TIP S 421 16.227 75.089 58.255 1.00 34.63 S O
ATOM 4434 OH2 TIP S 423 9.515 68.766 41.162 1.00 31.09 S O
ATOM 4435 OH2 TIP S 424 24.057 90.877 41.184 1.00 32.57 S O
ATOM 4436 OH2 TIP S 425 -23.421 85.321 34.874 1.00 40.73 S O
ATOM 4437 OH2 TIP S 426 -6.600 85.509 60.637 1.00 36.33 S O
ATOM 4438 OH2 TIP S 429 18.068 74.274 39.152 1.00 28.30 S O

Figure 7ZZZ

```
ATOM  4439  OH2 TIP S 430      0.216  72.088  29.280  1.00 34.77      S   O
ATOM  4440  OH2 TIP S 431     24.237  97.970  52.510  1.00 40.38      S   O
ATOM  4441  OH2 TIP S 433     16.496  61.776  20.380  1.00 31.74      S   O
ATOM  4442  OH2 TIP S 434     23.656  81.140  23.402  1.00 39.14      S   O
ATOM  4443  OH2 TIP S 435     45.512  70.376  23.767  1.00 38.06      S   O
ATOM  4444  OH2 TIP S 436      5.133  69.622  42.446  1.00 33.04      S   O
ATOM  4445  OH2 TIP S 440     23.692  79.457  34.661  1.00 40.65      S   O
ATOM  4446  OH2 TIP S 443     15.889  73.328  39.832  1.00 29.37      S   O
ATOM  4447  OH2 TIP S 444     -8.745  70.532  28.410  1.00 33.62      S   O
ATOM  4448  OH2 TIP S 446     32.260  78.506  13.999  1.00 45.13      S   O
ATOM  4449  OH2 TIP S 448     39.242  48.079  43.803  1.00 33.38      S   O
ATOM  4450  OH2 TIP S 449     34.559  75.768  22.405  1.00 31.84      S   O
ATOM  4451  OH2 TIP S 450     17.344  71.627  57.656  1.00 30.16      S   O
ATOM  4452  OH2 TIP S 453     17.850  55.704  64.074  1.00 41.95      S   O
ATOM  4453  OH2 TIP S 454     12.673  87.630  65.105  1.00 36.77      S   O
ATOM  4454  OH2 TIP S 455     18.393  73.689  58.998  1.00 35.69      S   O
ATOM  4455  OH2 TIP S 457     31.350  80.284  54.849  1.00 32.98      S   O
ATOM  4456  OH2 TIP S 459     31.948  64.117  63.134  1.00 33.16      S   O
ATOM  4457  OH2 TIP S 461     25.883  44.584  58.922  1.00 26.81      S   O
ATOM  4458  OH2 TIP S 462     15.411  75.744  38.970  1.00 38.18      S   O
ATOM  4459  OH2 TIP S 465     -6.694  85.996  51.462  1.00 39.03      S   O
ATOM  4460  OH2 TIP S 467     22.428  74.991  56.119  1.00 48.69      S   O
ATOM  4461  OH2 TIP S 472      7.409  68.343  43.765  1.00 40.63      S   O
ATOM  4462  OH2 TIP S 477      3.696  81.760  15.765  1.00 41.18      S   O
ATOM  4463  OH2 TIP S 478     36.353  75.696  51.865  1.00 40.40      S   O
ATOM  4464  OH2 TIP S 479     45.063  73.009  39.613  1.00 30.28      S   O
ATOM  4465  OH2 TIP S 480     35.167  68.155  64.949  1.00 36.43      S   O
ATOM  4466  OH2 TIP S 481     16.895  81.810  19.179  1.00 26.87      S   O
ATOM  4467  OH2 TIP S 482      9.338  64.581  19.670  1.00 47.45      S   O
ATOM  4468  OH2 TIP S 486     -4.142  97.143  32.076  1.00 40.89      S   O
ATOM  4469  OH2 TIP S 492      8.626 110.626  48.140  1.00 38.81      S   O
ATOM  4470  OH2 TIP S 493     10.344  52.396  54.552  1.00 40.72      S   O
ATOM  4471  OH2 TIP S 504     -6.927  90.936  52.736  1.00 32.58      S   O
ATOM  4472  OH2 TIP S 506     25.842  56.111  26.259  1.00 44.04      S   O
ATOM  4473  OH2 TIP S 511    -18.765  81.021  30.433  1.00 43.07      S   O
ATOM  4474  OH2 TIP S 514    -10.951  95.897  30.634  1.00 35.08      S   O
ATOM  4475  OH2 TIP S 515     18.239  91.555  29.988  1.00 35.01      S   O
ATOM  4476  OH2 TIP S 518     11.487  71.453  37.559  1.00 30.35      S   O
ATOM  4477  OH2 TIP S 519     -5.621  94.181  63.866  1.00 38.29      S   O
ATOM  4478  OH2 TIP S 522    -22.715  82.630  39.313  1.00 37.68      S   O
ATOM  4479  OH2 TIP S 523     13.832  92.634  28.634  1.00 42.35      S   O
ATOM  4480  OH2 TIP S 526     38.684  51.235  34.304  1.00 47.63      S   O
ATOM  4481  OH2 TIP S 528     36.575  81.337  36.652  1.00 30.20      S   O
ATOM  4482  OH2 TIP S 529     19.003  94.626  60.449  1.00 33.39      S   O
ATOM  4483  OH2 TIP S 532     45.213  64.758  44.484  1.00 43.40      S   O
ATOM  4484  OH2 TIP S 548     27.913  76.880  61.466  1.00 39.53      S   O
ATOM  4485  OH2 TIP S 550     -7.794  83.071  55.228  1.00 36.58      S   O
ATOM  4486  OH2 TIP S 551      6.856  87.791  20.410  1.00 45.36      S   O
ATOM  4487  OH2 TIP S 553     20.954  56.587  35.076  1.00 46.06      S   O
ATOM  4488  OH2 TIP S 559      6.709  95.476  37.577  1.00 37.67      S   O
ATOM  4489  OH2 TIP S 561     -5.111  70.585  43.095  1.00 36.29      S   O
ATOM  4490  OH2 TIP S 563     33.592  49.188  39.439  1.00 38.90      S   O
ATOM  4491  OH2 TIP S 567     24.268  93.456  38.866  1.00 41.73      S   O
ATOM  4492  OH2 TIP S 568     38.145  71.373  18.079  1.00 45.93      S   O
ATOM  4493  OH2 TIP S 570     10.042 104.897  57.893  1.00 35.94      S   O
ATOM  4494  OH2 TIP S 579      2.980  71.667  46.083  1.00 31.08      S   O
ATOM  4495  OH2 TIP S 588     42.992  48.494  46.292  1.00 42.53      S   O
ATOM  4496  OH2 TIP S 592      7.979 101.256  62.776  1.00 43.56      S   O
```

Figure 7AAAA

```
ATOM  4497  OH2 TIP S 596     40.729  51.604  40.374  1.00 44.86      S   O
ATOM  4498  OH2 TIP S 608     22.066  82.819  34.739  1.00 44.19      S   O
ATOM  4499  OH2 TIP S 612     23.253  56.890  32.646  1.00 37.91      S   O
ATOM  4500  OH2 TIP S 613     -4.126  71.281  39.257  1.00 40.53      S   O
ATOM  4501  OH2 TIP S 640     21.624 103.517  40.110  1.00 37.27      S   O
ATOM  4502  OH2 TIP S 648      5.614  70.703  52.258  1.00 52.65      S   O
ATOM  4503  OH2 TIP S 650     43.903  58.744  50.765  1.00 33.40      S   O
ATOM  4504  OH2 TIP S 655     -8.816  78.637  48.006  1.00 40.13      S   O
ATOM  4505  OH2 TIP S 656     -5.358  78.170  23.376  1.00 32.77      S   O
ATOM  4506  OH2 TIP S 657      3.160  70.067  31.591  1.00 35.22      S   O
ATOM  4507  OH2 TIP S 658     25.185  73.553  62.291  1.00 39.81      S   O
END
```

Figure 8A

```
REMARK coordinates from minimization and B-factor refinement
REMARK refinement resolution: 500.0 - 1.9 A
REMARK starting r= 0.2224 free_r= 0.2451
REMARK final   r= 0.2185 free_r= 0.2440
REMARK rmsd bonds= 0.006037  rmsd angles=  1.31354
REMARK B rmsd for bonded mainchain atoms=  0.696  target= 1.5
REMARK B rmsd for bonded sidechain atoms=  0.779  target= 2.0
REMARK B rmsd for angle mainchain atoms=  1.253  target= 2.0
REMARK B rmsd for angle sidechain atoms=  1.286  target= 2.5
REMARK target= mlf  final wa= 0.882454  final rweight=0.367395
REMARK cycles= 1 coordinate steps= 150 B-factor steps= 100
REMARK sg= C222(1) a= 83.05 b= 112.82 c= 74.12 alpha= 90 beta= 90 gamma= 90
REMARK topology file 1  : MSI_CNX_TOPPAR:protein.top
REMARK topology file 2  : gll.top
REMARK topology file 3  : MSI_CNX_TOPPAR:water.top
REMARK topology file 4  : MSI_CNX_TOPPAR:ion.top
REMARK topology file 5  : uma.top
REMARK parameter file 1  : MSI_CNX_TOPPAR:protein_rep.param
REMARK parameter file 2  : gll.par
REMARK parameter file 3  : MSI_CNX_TOPPAR:water_rep.param
REMARK parameter file 4  : MSI_CNX_TOPPAR:ion.param
REMARK parameter file 5  : uma.par
REMARK molecular structure file: automatic
REMARK input coordinates: cns8_reb.pdb
REMARK reflection file= ../../../mosflm_esrf/muri_trn_free_unique.fob
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.9
REMARK initial B-factor correction applied to fobs :
REMARK   B11=  3.991 B22= -8.126 B33=  4.136
REMARK   B12=  0.000 B13=  0.000 B23=  0.000
REMARK B-factor correction applied to coordinate array B:  -0.648
REMARK bulk solvent: (Mask) density level= 0.373583 e/A^3, B-factor= 48.6342 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range:    27807 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):  1265 (  4.5 % )
REMARK number of reflections rejected:                          0 (  0.0 % )
REMARK total number of reflections used:                    26542 ( 95.5 % )
REMARK number of reflections in working set:                25198 ( 90.6 % )
REMARK number of reflections in test set:                    1344 (  4.8 % )
CRYST1  83.050  112.820  74.120  90.00  90.00  90.00 C 2 2 21
REMARK FILENAME="refine.pdb"
REMARK DATE:Dec-11-2002  01:22:55      created by user: kemitl
REMARK Written by CNX VERSION:2000
ATOM      1  CB  PRO A  20     59.140  10.232  37.959  1.00 42.27       C
ATOM      2  CG  PRO A  20     60.118   9.060  37.995  1.00 42.63       C
ATOM      3  C   PRO A  20     58.220  11.395  35.947  1.00 41.62       C
ATOM      4  O   PRO A  20     59.154  12.042  35.457  1.00 41.55       O
ATOM      5  N   PRO A  20     59.374   9.210  35.773  1.00 42.45       N
ATOM      6  CD  PRO A  20     60.587   8.879  36.540  1.00 42.74       C
ATOM      7  CA  PRO A  20     58.468  10.041  36.605  1.00 42.13       C
ATOM      8  N   ARG A  21     56.961  11.820  35.938  1.00 40.77       N
ATOM      9  CA  ARG A  21     56.586  13.100  35.341  1.00 39.90       C
ATOM     10  CB  ARG A  21     55.792  12.875  34.053  1.00 41.14       C
ATOM     11  CG  ARG A  21     55.782  11.436  33.550  1.00 43.27       C
ATOM     12  CD  ARG A  21     54.592  10.646  34.098  1.00 44.85       C
ATOM     13  NE  ARG A  21     54.310   9.479  33.264  1.00 46.30       N
ATOM     14  CZ  ARG A  21     53.249   8.687  33.392  1.00 46.83       C
```

Figure 8B

```
ATOM   15 NH1 ARG A 21    52.338  8.918 34.332 1.00 46.85      N
ATOM   16 NH2 ARG A 21    53.095  7.661 32.562 1.00 47.39      N
ATOM   17 C   ARG A 21    55.738 13.891 36.327 1.00 38.37      C
ATOM   18 O   ARG A 21    55.175 13.321 37.261 1.00 38.35      O
ATOM   19 N   PRO A 22    55.635 15.217 36.134 1.00 36.71      N
ATOM   20 CD  PRO A 22    56.249 16.056 35.092 1.00 36.55      C
ATOM   21 CA  PRO A 22    54.834 16.026 37.053 1.00 35.10      C
ATOM   22 CB  PRO A 22    54.956 17.441 36.483 1.00 35.61      C
ATOM   23 CG  PRO A 22    55.312 17.226 35.048 1.00 36.83      C
ATOM   24 C   PRO A 22    53.392 15.548 37.177 1.00 33.33      C
ATOM   25 O   PRO A 22    52.737 15.204 36.193 1.00 33.12      O
ATOM   26 N   THR A 23    52.926 15.513 38.416 1.00 31.31      N
ATOM   27 CA  THR A 23    51.579 15.073 38.734 1.00 28.82      C
ATOM   28 CB  THR A 23    51.528 14.500 40.165 1.00 28.86      C
ATOM   29 OG1 THR A 23    52.345 13.324 40.230 1.00 29.00      O
ATOM   30 CG2 THR A 23    50.096 14.159 40.556 1.00 27.97      C
ATOM   31 C   THR A 23    50.615 16.241 38.626 1.00 27.22      C
ATOM   32 O   THR A 23    50.767 17.256 39.307 1.00 26.28      O
ATOM   33 N   VAL A 24    49.622 16.090 37.760 1.00 26.19      N
ATOM   34 CA  VAL A 24    48.623 17.123 37.564 1.00 25.17      C
ATOM   35 CB  VAL A 24    48.654 17.655 36.116 1.00 25.46      C
ATOM   36 CG1 VAL A 24    47.488 18.596 35.879 1.00 25.44      C
ATOM   37 CG2 VAL A 24    49.976 18.377 35.867 1.00 25.54      C
ATOM   38 C   VAL A 24    47.222 16.617 37.870 1.00 24.64      C
ATOM   39 O   VAL A 24    46.786 15.593 37.344 1.00 24.53      O
ATOM   40 N   LEU A 25    46.525 17.350 38.728 1.00 23.92      N
ATOM   41 CA  LEU A 25    45.163 17.004 39.093 1.00 23.77      C
ATOM   42 CB  LEU A 25    44.910 17.283 40.579 1.00 23.48      C
ATOM   43 CG  LEU A 25    43.437 17.288 41.007 1.00 24.15      C
ATOM   44 CD1 LEU A 25    42.844 15.882 40.865 1.00 23.60      C
ATOM   45 CD2 LEU A 25    43.322 17.779 42.455 1.00 24.84      C
ATOM   46 C   LEU A 25    44.189 17.840 38.279 1.00 23.16      C
ATOM   47 O   LEU A 25    44.368 19.048 38.143 1.00 22.71      O
ATOM   48 N   VAL A 26    43.177 17.183 37.723 1.00 23.08      N
ATOM   49 CA  VAL A 26    42.122 17.867 36.991 1.00 22.84      C
ATOM   50 CB  VAL A 26    42.017 17.396 35.525 1.00 23.04      C
ATOM   51 CG1 VAL A 26    40.884 18.138 34.832 1.00 22.64      C
ATOM   52 CG2 VAL A 26    43.346 17.665 34.788 1.00 22.73      C
ATOM   53 C   VAL A 26    40.852 17.482 37.764 1.00 23.16      C
ATOM   54 O   VAL A 26    40.520 16.295 37.876 1.00 23.27      O
ATOM   55 N   PHE A 27    40.172 18.485 38.315 1.00 22.82      N
ATOM   56 CA  PHE A 27    38.967 18.277 39.117 1.00 23.33      C
ATOM   57 CB  PHE A 27    39.168 18.865 40.518 1.00 23.65      C
ATOM   58 CG  PHE A 27    37.902 18.924 41.340 1.00 24.66      C
ATOM   59 CD1 PHE A 27    37.456 17.805 42.042 1.00 24.66      C
ATOM   60 CD2 PHE A 27    37.125 20.078 41.360 1.00 24.42      C
ATOM   61 CE1 PHE A 27    36.253 17.834 42.748 1.00 24.95      C
ATOM   62 CE2 PHE A 27    35.917 20.119 42.063 1.00 24.93      C
ATOM   63 CZ  PHE A 27    35.480 18.995 42.756 1.00 25.18      C
ATOM   64 C   PHE A 27    37.687 18.879 38.547 1.00 23.64      C
ATOM   65 O   PHE A 27    37.705 19.941 37.931 1.00 24.06      O
ATOM   66 N   ASP A 28    36.575 18.187 38.773 1.00 23.82      N
ATOM   67 CA  ASP A 28    35.253 18.651 38.358 1.00 23.43      C
ATOM   68 CB  ASP A 28    34.957 18.343 36.885 1.00 23.14      C
ATOM   69 CG  ASP A 28    33.602 18.896 36.443 1.00 23.57      C
ATOM   70 OD1 ASP A 28    32.893 18.244 35.646 1.00 23.23      O
ATOM   71 OD2 ASP A 28    33.239 19.998 36.903 1.00 24.14      O
ATOM   72 C   ASP A 28    34.226 17.924 39.202 1.00 23.59      C
```

Figure 8C

```
ATOM   73  O   ASP A 28    34.540  16.928  39.856  1.00 23.62      O
ATOM   74  N   SER A 29    32.996  18.421  39.179  1.00 23.49      N
ATOM   75  CA  SER A 29    31.904  17.800  39.913  1.00 23.63      C
ATOM   76  CB  SER A 29    30.717  18.757  39.969  1.00 23.55      C
ATOM   77  OG  SER A 29    30.313  19.099  38.657  1.00 24.80      O
ATOM   78  C   SER A 29    31.500  16.508  39.186  1.00 23.67      C
ATOM   79  O   SER A 29    31.007  15.564  39.804  1.00 23.60      O
ATOM   80  N   GLY A 30    31.721  16.471  37.874  1.00 23.60      N
ATOM   81  CA  GLY A 30    31.377  15.294  37.096  1.00 23.98      C
ATOM   82  C   GLY A 30    32.306  15.003  35.934  1.00 23.76      C
ATOM   83  O   GLY A 30    33.529  14.975  36.099  1.00 24.03      O
ATOM   84  N   VAL A 31    31.737  14.799  34.747  1.00 23.50      N
ATOM   85  CA  VAL A 31    32.536  14.491  33.566  1.00 23.42      C
ATOM   86  CB  VAL A 31    31.753  13.579  32.565  1.00 24.04      C
ATOM   87  CG1 VAL A 31    31.393  12.253  33.231  1.00 24.26      C
ATOM   88  CG2 VAL A 31    30.484  14.277  32.079  1.00 24.22      C
ATOM   89  C   VAL A 31    33.054  15.712  32.792  1.00 23.39      C
ATOM   90  O   VAL A 31    33.948  15.576  31.960  1.00 22.93      O
ATOM   91  N   GLY A 32    32.503  16.892  33.062  1.00 23.03      N
ATOM   92  CA  GLY A 32    32.933  18.083  32.341  1.00 23.53      C
ATOM   93  C   GLY A 32    34.434  18.316  32.374  1.00 23.94      C
ATOM   94  O   GLY A 32    35.018  18.803  31.406  1.00 23.61      O
ATOM   95  N   GLY A 33    35.058  17.971  33.496  1.00 23.88      N
ATOM   96  CA  GLY A 33    36.492  18.149  33.641  1.00 24.00      C
ATOM   97  C   GLY A 33    37.272  17.468  32.537  1.00 24.04      C
ATOM   98  O   GLY A 33    38.347  17.921  32.174  1.00 24.11      O
ATOM   99  N   LEU A 34    36.720  16.389  31.990  1.00 24.29      N
ATOM   100 CA  LEU A 34    37.377  15.653  30.923  1.00 24.12      C
ATOM   101 CB  LEU A 34    36.586  14.384  30.589  1.00 24.26      C
ATOM   102 CG  LEU A 34    36.559  13.331  31.703  1.00 24.52      C
ATOM   103 CD1 LEU A 34    35.609  12.209  31.311  1.00 24.48      C
ATOM   104 CD2 LEU A 34    37.969  12.795  31.940  1.00 24.92      C
ATOM   105 C   LEU A 34    37.586  16.474  29.652  1.00 23.95      C
ATOM   106 O   LEU A 34    38.524  16.212  28.907  1.00 24.13      O
ATOM   107 N   SER A 35    36.729  17.461  29.394  1.00 23.76      N
ATOM   108 CA  SER A 35    36.916  18.270  28.191  1.00 24.21      C
ATOM   109 CB  SER A 35    35.694  19.159  27.909  1.00 23.45      C
ATOM   110 OG  SER A 35    35.531  20.175  28.886  1.00 23.98      O
ATOM   111 C   SER A 35    38.173  19.137  28.347  1.00 24.34      C
ATOM   112 O   SER A 35    38.910  19.357  27.383  1.00 24.46      O
ATOM   113 N   VAL A 36    38.416  19.611  29.564  1.00 24.57      N
ATOM   114 CA  VAL A 36    39.582  20.444  29.847  1.00 25.04      C
ATOM   115 CB  VAL A 36    39.445  21.160  31.211  1.00 25.08      C
ATOM   116 CG1 VAL A 36    40.682  22.024  31.482  1.00 25.12      C
ATOM   117 CG2 VAL A 36    38.188  22.020  31.212  1.00 25.41      C
ATOM   118 C   VAL A 36    40.824  19.572  29.863  1.00 25.61      C
ATOM   119 O   VAL A 36    41.869  19.935  29.313  1.00 25.10      O
ATOM   120 N   TYR A 37    40.704  18.407  30.494  1.00 26.15      N
ATOM   121 CA  TYR A 37    41.816  17.478  30.550  1.00 26.62      C
ATOM   122 CB  TYR A 37    41.427  16.236  31.367  1.00 26.04      C
ATOM   123 CG  TYR A 37    42.210  14.999  31.006  1.00 26.11      C
ATOM   124 CD1 TYR A 37    41.696  14.065  30.106  1.00 26.04      C
ATOM   125 CE1 TYR A 37    42.431  12.937  29.737  1.00 26.06      C
ATOM   126 CD2 TYR A 37    43.483  14.777  31.532  1.00 26.28      C
ATOM   127 CE2 TYR A 37    44.227  13.654  31.167  1.00 26.29      C
ATOM   128 CZ  TYR A 37    43.694  12.742  30.274  1.00 26.29      C
ATOM   129 OH  TYR A 37    44.414  11.627  29.922  1.00 26.91      O
ATOM   130 C   TYR A 37    42.243  17.072  29.139  1.00 27.35      C
```

Figure 8D

```
ATOM    131  O   TYR A  37      43.431  16.998  28.840  1.00 27.42           O
ATOM    132  N   ASP A  38      41.270  16.815  28.274  1.00 28.14           N
ATOM    133  CA  ASP A  38      41.554  16.403  26.906  1.00 29.79           C
ATOM    134  CB  ASP A  38      40.234  16.233  26.149  1.00 30.37           C
ATOM    135  CG  ASP A  38      40.355  15.321  24.945  1.00 31.87           C
ATOM    136  OD1 ASP A  38      41.285  14.487  24.904  1.00 32.39           O
ATOM    137  OD2 ASP A  38      39.495  15.427  24.039  1.00 32.89           O
ATOM    138  C   ASP A  38      42.472  17.411  26.200  1.00 30.27           C
ATOM    139  O   ASP A  38      43.406  17.018  25.500  1.00 30.51           O
ATOM    140  N   GLU A  39      42.213  18.702  26.399  1.00 30.88           N
ATOM    141  CA  GLU A  39      43.032  19.759  25.799  1.00 32.05           C
ATOM    142  CB  GLU A  39      42.367  21.123  25.992  1.00 32.93           C
ATOM    143  CG  GLU A  39      41.075  21.325  25.219  1.00 35.19           C
ATOM    144  CD  GLU A  39      41.310  21.703  23.766  1.00 36.77           C
ATOM    145  OE1 GLU A  39      40.316  21.968  23.056  1.00 38.63           O
ATOM    146  OE2 GLU A  39      42.481  21.743  23.333  1.00 37.13           O
ATOM    147  C   GLU A  39      44.417  19.786  26.447  1.00 32.29           C
ATOM    148  O   GLU A  39      45.435  19.941  25.772  1.00 31.60           O
ATOM    149  N   ILE A  40      44.454  19.640  27.765  1.00 32.60           N
ATOM    150  CA  ILE A  40      45.726  19.646  28.472  1.00 33.11           C
ATOM    151  CB  ILE A  40      45.517  19.585  29.998  1.00 32.73           C
ATOM    152  CG2 ILE A  40      46.867  19.494  30.709  1.00 32.95           C
ATOM    153  CG1 ILE A  40      44.750  20.824  30.468  1.00 32.28           C
ATOM    154  CD1 ILE A  40      44.401  20.809  31.947  1.00 32.55           C
ATOM    155  C   ILE A  40      46.623  18.486  28.040  1.00 33.95           C
ATOM    156  O   ILE A  40      47.806  18.688  27.753  1.00 33.92           O
ATOM    157  N   ARG A  41      46.072  17.275  27.982  1.00 34.92           N
ATOM    158  CA  ARG A  41      46.872  16.118  27.593  1.00 36.38           C
ATOM    159  CB  ARG A  41      46.114  14.805  27.815  1.00 36.95           C
ATOM    160  CG  ARG A  41      44.970  14.556  26.850  1.00 38.65           C
ATOM    161  CD  ARG A  41      44.714  13.060  26.676  1.00 40.05           C
ATOM    162  NE  ARG A  41      43.499  12.807  25.905  1.00 41.30           N
ATOM    163  CZ  ARG A  41      43.076  11.600  25.541  1.00 41.65           C
ATOM    164  NH1 ARG A  41      43.770  10.518  25.872  1.00 41.91           N
ATOM    165  NH2 ARG A  41      41.952  11.475  24.847  1.00 42.04           N
ATOM    166  C   ARG A  41      47.324  16.188  26.141  1.00 37.23           C
ATOM    167  O   ARG A  41      48.347  15.618  25.780  1.00 36.68           O
ATOM    168  N   HIS A  42      46.554  16.870  25.303  1.00 38.38           N
ATOM    169  CA  HIS A  42      46.935  16.990  23.905  1.00 39.98           C
ATOM    170  CB  HIS A  42      45.803  17.637  23.102  1.00 40.97           C
ATOM    171  CG  HIS A  42      46.096  17.757  21.640  1.00 42.48           C
ATOM    172  CD2 HIS A  42      45.580  17.104  20.571  1.00 43.17           C
ATOM    173  ND1 HIS A  42      47.032  18.634  21.137  1.00 43.19           N
ATOM    174  CE1 HIS A  42      47.080  18.519  19.821  1.00 43.48           C
ATOM    175  NE2 HIS A  42      46.208  17.597  19.452  1.00 43.37           N
ATOM    176  C   HIS A  42      48.207  17.836  23.822  1.00 40.26           C
ATOM    177  O   HIS A  42      49.053  17.625  22.955  1.00 40.52           O
ATOM    178  N   LEU A  43      48.341  18.783  24.747  1.00 40.38           N
ATOM    179  CA  LEU A  43      49.500  19.662  24.795  1.00 40.54           C
ATOM    180  CB  LEU A  43      49.087  21.020  25.372  1.00 40.84           C
ATOM    181  CG  LEU A  43      50.118  22.150  25.372  1.00 40.88           C
ATOM    182  CD1 LEU A  43      50.521  22.468  23.935  1.00 41.44           C
ATOM    183  CD2 LEU A  43      49.533  23.386  26.043  1.00 40.98           C
ATOM    184  C   LEU A  43      50.638  19.065  25.631  1.00 40.74           C
ATOM    185  O   LEU A  43      51.812  19.224  25.299  1.00 40.80           O
ATOM    186  N   LEU A  44      50.284  18.379  26.715  1.00 40.77           N
ATOM    187  CA  LEU A  44      51.263  17.759  27.615  1.00 40.94           C
ATOM    188  CB  LEU A  44      51.281  18.515  28.942  1.00 40.98           C
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Figure 8E

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ATOM   189  CG  LEU A  44      51.493  20.023  28.814  1.00 40.82           C
ATOM   190  CD1 LEU A  44      51.011  20.721  30.066  1.00 40.73           C
ATOM   191  CD2 LEU A  44      52.964  20.307  28.550  1.00 41.26           C
ATOM   192  C   LEU A  44      50.841  16.310  27.841  1.00 41.15           C
ATOM   193  O   LEU A  44      50.325  15.955  28.903  1.00 41.15           O
ATOM   194  N   PRO A  45      51.075  15.445  26.843  1.00 41.22           N
ATOM   195  CD  PRO A  45      51.677  15.806  25.545  1.00 41.47           C
ATOM   196  CA  PRO A  45      50.725  14.021  26.873  1.00 41.13           C
ATOM   197  CB  PRO A  45      50.900  13.604  25.413  1.00 41.22           C
ATOM   198  CG  PRO A  45      52.040  14.456  24.968  1.00 41.02           C
ATOM   199  C   PRO A  45      51.418  13.044  27.826  1.00 41.10           C
ATOM   200  O   PRO A  45      50.885  11.961  28.077  1.00 41.10           O
ATOM   201  N   ASP A  46      52.576  13.400  28.373  1.00 40.74           N
ATOM   202  CA  ASP A  46      53.280  12.454  29.240  1.00 40.25           C
ATOM   203  CB  ASP A  46      54.765  12.400  28.854  1.00 41.61           C
ATOM   204  CG  ASP A  46      54.974  12.058  27.391  1.00 43.12           C
ATOM   205  OD1 ASP A  46      54.498  10.985  26.956  1.00 43.83           O
ATOM   206  OD2 ASP A  46      55.618  12.863  26.676  1.00 44.38           O
ATOM   207  C   ASP A  46      53.176  12.666  30.749  1.00 38.90           C
ATOM   208  O   ASP A  46      53.812  11.941  31.511  1.00 39.20           O
ATOM   209  N   LEU A  47      52.381  13.636  31.185  1.00 36.81           N
ATOM   210  CA  LEU A  47      52.249  13.907  32.614  1.00 34.74           C
ATOM   211  CB  LEU A  47      51.450  15.194  32.833  1.00 34.94           C
ATOM   212  CG  LEU A  47      51.913  16.438  32.077  1.00 34.69           C
ATOM   213  CD1 LEU A  47      51.018  17.604  32.434  1.00 35.28           C
ATOM   214  CD2 LEU A  47      53.358  16.746  32.428  1.00 35.67           C
ATOM   215  C   LEU A  47      51.564  12.774  33.364  1.00 33.31           C
ATOM   216  O   LEU A  47      50.968  11.881  32.758  1.00 33.06           O
ATOM   217  N   HIS A  48      51.678  12.800  34.689  1.00 31.91           N
ATOM   218  CA  HIS A  48      51.013  11.808  35.530  1.00 30.54           C
ATOM   219  CB  HIS A  48      51.794  11.524  36.814  1.00 30.57           C
ATOM   220  CG  HIS A  48      51.017  10.729  37.822  1.00 30.87           C
ATOM   221  CD2 HIS A  48      50.251   9.620  37.685  1.00 30.97           C
ATOM   222  ND1 HIS A  48      50.986  11.050  39.163  1.00 31.68           N
ATOM   223  CE1 HIS A  48      50.236  10.173  39.808  1.00 31.33           C
ATOM   224  NE2 HIS A  48      49.778   9.295  38.933  1.00 31.22           N
ATOM   225  C   HIS A  48      49.704  12.490  35.900  1.00 29.55           C
ATOM   226  O   HIS A  48      49.668  13.331  36.802  1.00 29.03           O
ATOM   227  N   TYR A  49      48.641  12.139  35.194  1.00 28.24           N
ATOM   228  CA  TYR A  49      47.349  12.754  35.441  1.00 27.76           C
ATOM   229  CB  TYR A  49      46.555  12.878  34.135  1.00 28.09           C
ATOM   230  CG  TYR A  49      47.108  13.881  33.145  1.00 28.48           C
ATOM   231  CD1 TYR A  49      47.890  13.471  32.066  1.00 28.86           C
ATOM   232  CE1 TYR A  49      48.375  14.395  31.124  1.00 29.12           C
ATOM   233  CD2 TYR A  49      46.823  15.242  33.275  1.00 28.88           C
ATOM   234  CE2 TYR A  49      47.301  16.173  32.350  1.00 29.31           C
ATOM   235  CZ  TYR A  49      48.075  15.741  31.275  1.00 29.63           C
ATOM   236  OH  TYR A  49      48.527  16.665  30.353  1.00 29.75           O
ATOM   237  C   TYR A  49      46.477  12.040  36.463  1.00 27.00           C
ATOM   238  O   TYR A  49      46.433  10.808  36.533  1.00 26.57           O
ATOM   239  N   ILE A  50      45.791  12.844  37.259  1.00 25.98           N
ATOM   240  CA  ILE A  50      44.854  12.340  38.243  1.00 24.91           C
ATOM   241  CB  ILE A  50      45.259  12.705  39.682  1.00 24.96           C
ATOM   242  CG2 ILE A  50      44.167  12.253  40.654  1.00 23.79           C
ATOM   243  CG1 ILE A  50      46.598  12.054  40.041  1.00 24.11           C
ATOM   244  CD1 ILE A  50      47.213  12.622  41.313  1.00 24.92           C
ATOM   245  C   ILE A  50      43.560  13.071  37.933  1.00 24.67           C
ATOM   246  O   ILE A  50      43.536  14.305  37.900  1.00 24.39           O
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Figure 8F

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ATOM   247 N   TYR A 51    42.498  12.321  37.671  1.00 24.20      N
ATOM   248 CA  TYR A 51    41.205  12.933  37.413  1.00 24.34      C
ATOM   249 CB  TYR A 51    40.549  12.369  36.148  1.00 24.65      C
ATOM   250 CG  TYR A 51    39.285  13.123  35.766  1.00 25.11      C
ATOM   251 CD1 TYR A 51    38.018  12.626  36.076  1.00 25.28      C
ATOM   252 CE1 TYR A 51    36.860  13.369  35.793  1.00 25.75      C
ATOM   253 CD2 TYR A 51    39.366  14.376  35.157  1.00 25.76      C
ATOM   254 CE2 TYR A 51    38.220  15.122  34.867  1.00 25.82      C
ATOM   255 CZ  TYR A 51    36.974  14.620  35.189  1.00 26.04      C
ATOM   256 OH  TYR A 51    35.856  15.394  34.926  1.00 25.60      O
ATOM   257 C   TYR A 51    40.337  12.612  38.616  1.00 24.47      C
ATOM   258 O   TYR A 51    40.221  11.451  39.014  1.00 24.67      O
ATOM   259 N   ALA A 52    39.740  13.637  39.208  1.00 24.11      N
ATOM   260 CA  ALA A 52    38.878  13.425  40.363  1.00 23.89      C
ATOM   261 CB  ALA A 52    39.533  13.994  41.619  1.00 23.82      C
ATOM   262 C   ALA A 52    37.533  14.090  40.131  1.00 23.96      C
ATOM   263 O   ALA A 52    37.466  15.253  39.723  1.00 23.07      O
ATOM   264 N   PHE A 53    36.461  13.347  40.372  1.00 23.37      N
ATOM   265 CA  PHE A 53    35.132  13.906  40.208  1.00 23.51      C
ATOM   266 CB  PHE A 53    34.474  13.388  38.909  1.00 23.73      C
ATOM   267 CG  PHE A 53    34.310  11.889  38.838  1.00 24.04      C
ATOM   268 CD1 PHE A 53    33.054  11.309  39.007  1.00 23.82      C
ATOM   269 CD2 PHE A 53    35.398  11.066  38.559  1.00 24.45      C
ATOM   270 CE1 PHE A 53    32.882   9.929  38.895  1.00 24.38      C
ATOM   271 CE2 PHE A 53    35.242   9.679  38.445  1.00 24.39      C
ATOM   272 CZ  PHE A 53    33.978   9.111  38.614  1.00 24.35      C
ATOM   273 C   PHE A 53    34.276  13.625  41.444  1.00 23.79      C
ATOM   274 O   PHE A 53    34.305  12.528  42.013  1.00 22.86      O
ATOM   275 N   ASP A 54    33.533  14.642  41.868  1.00 23.79      N
ATOM   276 CA  ASP A 54    32.682  14.541  43.051  1.00 24.06      C
ATOM   277 CB  ASP A 54    32.563  15.916  43.714  1.00 23.89      C
ATOM   278 CG  ASP A 54    31.963  15.840  45.109  1.00 23.89      C
ATOM   279 OD1 ASP A 54    31.577  14.727  45.538  1.00 22.90      O
ATOM   280 OD2 ASP A 54    31.880  16.894  45.772  1.00 23.05      O
ATOM   281 C   ASP A 54    31.289  14.002  42.734  1.00 24.18      C
ATOM   282 O   ASP A 54    30.312  14.750  42.734  1.00 23.82      O
ATOM   283 N   ASN A 55    31.191  12.698  42.488  1.00 24.17      N
ATOM   284 CA  ASN A 55    29.905  12.103  42.170  1.00 25.09      C
ATOM   285 CB  ASN A 55    30.090  10.674  41.631  1.00 25.26      C
ATOM   286 CG  ASN A 55    30.731   9.737  42.639  1.00 25.36      C
ATOM   287 OD1 ASN A 55    31.791  10.028  43.201  1.00 24.79      O
ATOM   288 ND2 ASN A 55    30.092   8.592  42.864  1.00 25.74      N
ATOM   289 C   ASN A 55    28.970  12.110  43.376  1.00 25.56      C
ATOM   290 O   ASN A 55    27.770  11.915  43.226  1.00 25.79      O
ATOM   291 N   VAL A 56    29.520  12.362  44.561  1.00 25.66      N
ATOM   292 CA  VAL A 56    28.731  12.405  45.794  1.00 26.16      C
ATOM   293 CB  VAL A 56    29.642  12.231  47.043  1.00 26.47      C
ATOM   294 CG1 VAL A 56    28.888  12.614  48.320  1.00 26.82      C
ATOM   295 CG2 VAL A 56    30.112  10.785  47.140  1.00 26.75      C
ATOM   296 C   VAL A 56    27.930  13.704  45.950  1.00 26.34      C
ATOM   297 O   VAL A 56    26.779  13.683  46.395  1.00 26.27      O
ATOM   298 N   ALA A 57    28.528  14.831  45.576  1.00 25.69      N
ATOM   299 CA  ALA A 57    27.846  16.106  45.723  1.00 25.62      C
ATOM   300 CB  ALA A 57    28.721  17.072  46.509  1.00 25.61      C
ATOM   301 C   ALA A 57    27.399  16.740  44.405  1.00 25.80      C
ATOM   302 O   ALA A 57    26.813  17.820  44.406  1.00 25.99      O
ATOM   303 N   PHE A 58    27.675  16.079  43.284  1.00 25.66      N
ATOM   304 CA  PHE A 58    27.242  16.595  41.984  1.00 25.94      C
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Figure 8G

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ATOM   305  CB  PHE A  58      27.689  15.659  40.856  1.00 25.77           C
ATOM   306  CG  PHE A  58      27.101  16.006  39.517  1.00 26.33           C
ATOM   307  CD1 PHE A  58      27.725  16.933  38.684  1.00 26.01           C
ATOM   308  CD2 PHE A  58      25.892  15.445  39.112  1.00 26.14           C
ATOM   309  CE1 PHE A  58      27.152  17.300  37.467  1.00 26.79           C
ATOM   310  CE2 PHE A  58      25.308  15.807  37.893  1.00 27.07           C
ATOM   311  CZ  PHE A  58      25.938  16.735  37.071  1.00 27.22           C
ATOM   312  C   PHE A  58      25.714  16.601  42.045  1.00 26.23           C
ATOM   313  O   PHE A  58      25.123  15.651  42.555  1.00 26.27           O
ATOM   314  N   PRO A  59      25.053  17.645  41.507  1.00 26.87           N
ATOM   315  CD  PRO A  59      23.589  17.565  41.316  1.00 27.24           C
ATOM   316  CA  PRO A  59      25.591  18.836  40.838  1.00 27.09           C
ATOM   317  CB  PRO A  59      24.484  19.195  39.850  1.00 27.32           C
ATOM   318  CG  PRO A  59      23.257  18.898  40.647  1.00 27.45           C
ATOM   319  C   PRO A  59      25.902  19.993  41.788  1.00 27.44           C
ATOM   320  O   PRO A  59      25.197  20.214  42.776  1.00 26.87           O
ATOM   321  N   TYR A  60      26.968  20.725  41.476  1.00 28.08           N
ATOM   322  CA  TYR A  60      27.395  21.870  42.277  1.00 29.46           C
ATOM   323  CB  TYR A  60      28.873  22.182  41.988  1.00 28.52           C
ATOM   324  CG  TYR A  60      29.887  21.318  42.725  1.00 27.75           C
ATOM   325  CD1 TYR A  60      29.520  20.113  43.339  1.00 27.37           C
ATOM   326  CE1 TYR A  60      30.475  19.317  44.006  1.00 26.91           C
ATOM   327  CD2 TYR A  60      31.228  21.708  42.794  1.00 27.09           C
ATOM   328  CE2 TYR A  60      32.178  20.932  43.450  1.00 27.19           C
ATOM   329  CZ  TYR A  60      31.802  19.739  44.054  1.00 27.07           C
ATOM   330  OH  TYR A  60      32.758  18.982  44.698  1.00 25.80           O
ATOM   331  C   TYR A  60      26.539  23.119  41.991  1.00 30.92           C
ATOM   332  O   TYR A  60      26.389  23.993  42.849  1.00 30.67           O
ATOM   333  N   GLY A  61      25.981  23.190  40.785  1.00 33.00           N
ATOM   334  CA  GLY A  61      25.165  24.332  40.400  1.00 35.24           C
ATOM   335  C   GLY A  61      24.126  24.770  41.418  1.00 37.04           C
ATOM   336  O   GLY A  61      23.892  25.965  41.601  1.00 37.85           O
ATOM   337  N   GLU A  62      23.512  23.803  42.089  1.00 38.35           N
ATOM   338  CA  GLU A  62      22.479  24.069  43.088  1.00 39.52           C
ATOM   339  CB  GLU A  62      21.559  22.852  43.183  1.00 41.20           C
ATOM   340  CG  GLU A  62      22.340  21.562  43.450  1.00 43.11           C
ATOM   341  CD  GLU A  62      21.455  20.385  43.790  1.00 44.30           C
ATOM   342  OE1 GLU A  62      20.626  19.994  42.931  1.00 45.50           O
ATOM   343  OE2 GLU A  62      21.590  19.850  44.917  1.00 44.82           O
ATOM   344  C   GLU A  62      23.026  24.374  44.487  1.00 39.48           C
ATOM   345  O   GLU A  62      22.459  25.187  45.226  1.00 40.03           O
ATOM   346  N   LYS A  63      24.123  23.708  44.833  1.00 38.32           N
ATOM   347  CA  LYS A  63      24.772  23.827  46.135  1.00 37.54           C
ATOM   348  CB  LYS A  63      26.033  22.956  46.148  1.00 36.71           C
ATOM   349  CG  LYS A  63      25.795  21.494  45.761  1.00 36.22           C
ATOM   350  CD  LYS A  63      24.954  20.758  46.796  1.00 35.50           C
ATOM   351  CE  LYS A  63      24.888  19.257  46.509  1.00 34.57           C
ATOM   352  NZ  LYS A  63      24.287  18.933  45.180  1.00 33.47           N
ATOM   353  C   LYS A  63      25.130  25.233  46.623  1.00 37.13           C
ATOM   354  O   LYS A  63      25.354  26.153  45.833  1.00 37.17           O
ATOM   355  N   SER A  64      25.180  25.376  47.944  1.00 36.87           N
ATOM   356  CA  SER A  64      25.531  26.637  48.590  1.00 36.73           C
ATOM   357  CB  SER A  64      25.270  26.553  50.096  1.00 36.69           C
ATOM   358  OG  SER A  64      23.936  26.162  50.370  1.00 37.39           O
ATOM   359  C   SER A  64      27.017  26.869  48.360  1.00 36.81           C
ATOM   360  O   SER A  64      27.801  25.915  48.358  1.00 36.64           O
ATOM   361  N   GLU A  65      27.410  28.125  48.177  1.00 36.66           N
ATOM   362  CA  GLU A  65      28.813  28.439  47.947  1.00 36.97           C
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Figure 8H

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ATOM   363 CB  GLU A 65     28.985 29.926 47.611 1.00 38.23      C
ATOM   364 CG  GLU A 65     28.742 30.243 46.138 1.00 40.25      C
ATOM   365 CD  GLU A 65     28.841 31.730 45.815 1.00 42.02      C
ATOM   366 OE1 GLU A 65     29.763 32.403 46.336 1.00 43.02      O
ATOM   367 OE2 GLU A 65     28.006 32.223 45.023 1.00 43.06      O
ATOM   368 C   GLU A 65     29.702 28.050 49.122 1.00 36.16      C
ATOM   369 O   GLU A 65     30.831 27.606 48.917 1.00 36.24      O
ATOM   370 N   ALA A 66     29.198 28.202 50.345 1.00 35.06      N
ATOM   371 CA  ALA A 66     29.972 27.845 51.536 1.00 34.39      C
ATOM   372 CB  ALA A 66     29.191 28.190 52.794 1.00 34.26      C
ATOM   373 C   ALA A 66     30.317 26.348 51.522 1.00 33.80      C
ATOM   374 O   ALA A 66     31.420 25.943 51.903 1.00 33.49      O
ATOM   375 N   PHE A 67     29.367 25.528 51.087 1.00 32.84      N
ATOM   376 CA  PHE A 67     29.598 24.091 51.009 1.00 31.99      C
ATOM   377 CB  PHE A 67     28.308 23.339 50.657 1.00 31.83      C
ATOM   378 CG  PHE A 67     28.550 21.930 50.191 1.00 31.22      C
ATOM   379 CD1 PHE A 67     28.891 20.928 51.098 1.00 31.15      C
ATOM   380 CD2 PHE A 67     28.526 21.625 48.834 1.00 31.38      C
ATOM   381 CE1 PHE A 67     29.211 19.639 50.657 1.00 30.97      C
ATOM   382 CE2 PHE A 67     28.846 20.337 48.384 1.00 31.33      C
ATOM   383 CZ  PHE A 67     29.189 19.346 49.301 1.00 30.62      C
ATOM   384 C   PHE A 67     30.643 23.796 49.936 1.00 31.40      C
ATOM   385 O   PHE A 67     31.613 23.082 50.186 1.00 31.16      O
ATOM   386 N   ILE A 68     30.433 24.350 48.744 1.00 30.67      N
ATOM   387 CA  ILE A 68     31.338 24.139 47.618 1.00 30.11      C
ATOM   388 CB  ILE A 68     30.926 25.003 46.394 1.00 29.93      C
ATOM   389 CG2 ILE A 68     31.983 24.902 45.294 1.00 29.25      C
ATOM   390 CG1 ILE A 68     29.568 24.533 45.858 1.00 30.20      C
ATOM   391 CD1 ILE A 68     29.116 25.245 44.591 1.00 30.32      C
ATOM   392 C   ILE A 68     32.809 24.414 47.944 1.00 30.38      C
ATOM   393 O   ILE A 68     33.679 23.591 47.649 1.00 29.53      O
ATOM   394 N   VAL A 69     33.092 25.567 48.545 1.00 30.39      N
ATOM   395 CA  VAL A 69     34.470 25.907 48.886 1.00 30.68      C
ATOM   396 CB  VAL A 69     34.557 27.290 49.579 1.00 31.33      C
ATOM   397 CG1 VAL A 69     35.998 27.578 49.994 1.00 31.13      C
ATOM   398 CG2 VAL A 69     34.052 28.376 48.631 1.00 31.78      C
ATOM   399 C   VAL A 69     35.085 24.851 49.801 1.00 30.46      C
ATOM   400 O   VAL A 69     36.175 24.349 49.523 1.00 30.83      O
ATOM   401 N   GLU A 70     34.379 24.508 50.878 1.00 29.88      N
ATOM   402 CA  GLU A 70     34.869 23.518 51.834 1.00 30.07      C
ATOM   403 CB  GLU A 70     33.899 23.369 53.016 1.00 31.73      C
ATOM   404 CG  GLU A 70     33.763 24.597 53.925 1.00 35.37      C
ATOM   405 CD  GLU A 70     35.085 25.046 54.534 1.00 37.49      C
ATOM   406 OE1 GLU A 70     35.894 24.179 54.938 1.00 39.42      O
ATOM   407 OE2 GLU A 70     35.314 26.273 54.619 1.00 39.33      O
ATOM   408 C   GLU A 70     35.064 22.148 51.191 1.00 28.57      C
ATOM   409 O   GLU A 70     36.051 21.452 51.458 1.00 28.03      O
ATOM   410 N   ARG A 71     34.109 21.768 50.354 1.00 26.83      N
ATOM   411 CA  ARG A 71     34.140 20.478 49.677 1.00 25.52      C
ATOM   412 CB  ARG A 71     32.827 20.259 48.919 1.00 25.00      C
ATOM   413 CG  ARG A 71     32.717 18.924 48.195 1.00 24.55      C
ATOM   414 CD  ARG A 71     32.741 17.739 49.156 1.00 24.30      C
ATOM   415 NE  ARG A 71     32.481 16.490 48.437 1.00 24.43      N
ATOM   416 CZ  ARG A 71     32.569 15.278 48.973 1.00 24.76      C
ATOM   417 NH1 ARG A 71     32.915 15.130 50.248 1.00 24.34      N
ATOM   418 NH2 ARG A 71     32.321 14.210 48.227 1.00 24.54      N
ATOM   419 C   ARG A 71     35.320 20.345 48.722 1.00 24.66      C
ATOM   420 O   ARG A 71     36.044 19.352 48.769 1.00 24.09      O
```

Figure 8I

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ATOM   421  N   VAL A  72     35.521  21.342  47.863  1.00 23.70      N
ATOM   422  CA  VAL A  72     36.622  21.279  46.909  1.00 23.69      C
ATOM   423  CB  VAL A  72     36.537  22.428  45.883  1.00 23.55      C
ATOM   424  CG1 VAL A  72     37.697  22.337  44.904  1.00 23.48      C
ATOM   425  CG2 VAL A  72     35.206  22.337  45.125  1.00 24.07      C
ATOM   426  C   VAL A  72     37.976  21.301  47.623  1.00 23.44      C
ATOM   427  O   VAL A  72     38.907  20.607  47.216  1.00 23.28      O
ATOM   428  N   VAL A  73     38.085  22.088  48.686  1.00 23.43      N
ATOM   429  CA  VAL A  73     39.326  22.139  49.451  1.00 23.42      C
ATOM   430  CB  VAL A  73     39.264  23.209  50.571  1.00 24.16      C
ATOM   431  CG1 VAL A  73     40.438  23.033  51.540  1.00 24.47      C
ATOM   432  CG2 VAL A  73     39.316  24.604  49.964  1.00 24.03      C
ATOM   433  C   VAL A  73     39.578  20.755  50.076  1.00 23.35      C
ATOM   434  O   VAL A  73     40.707  20.277  50.094  1.00 23.23      O
ATOM   435  N   ALA A  74     38.527  20.108  50.575  1.00 22.61      N
ATOM   436  CA  ALA A  74     38.679  18.782  51.179  1.00 22.36      C
ATOM   437  CB  ALA A  74     37.382  18.355  51.870  1.00 22.18      C
ATOM   438  C   ALA A  74     39.085  17.736  50.132  1.00 22.47      C
ATOM   439  O   ALA A  74     39.916  16.867  50.400  1.00 21.70      O
ATOM   440  N   ILE A  75     38.499  17.806  48.940  1.00 22.12      N
ATOM   441  CA  ILE A  75     38.857  16.845  47.911  1.00 22.33      C
ATOM   442  CB  ILE A  75     37.898  16.942  46.695  1.00 22.09      C
ATOM   443  CG2 ILE A  75     38.439  16.106  45.531  1.00 21.64      C
ATOM   444  CG1 ILE A  75     36.502  16.455  47.107  1.00 22.35      C
ATOM   445  CD1 ILE A  75     35.414  16.664  46.055  1.00 21.88      C
ATOM   446  C   ILE A  75     40.319  17.017  47.460  1.00 22.41      C
ATOM   447  O   ILE A  75     41.038  16.033  47.306  1.00 22.76      O
ATOM   448  N   VAL A  76     40.770  18.253  47.259  1.00 22.98      N
ATOM   449  CA  VAL A  76     42.157  18.464  46.831  1.00 22.84      C
ATOM   450  CB  VAL A  76     42.436  19.945  46.478  1.00 23.18      C
ATOM   451  CG1 VAL A  76     43.922  20.122  46.125  1.00 23.17      C
ATOM   452  CG2 VAL A  76     41.557  20.376  45.294  1.00 22.52      C
ATOM   453  C   VAL A  76     43.106  18.030  47.951  1.00 23.01      C
ATOM   454  O   VAL A  76     44.206  17.542  47.706  1.00 22.66      O
ATOM   455  N   THR A  77     42.672  18.207  49.190  1.00 23.25      N
ATOM   456  CA  THR A  77     43.482  17.802  50.329  1.00 23.42      C
ATOM   457  CB  THR A  77     42.804  18.220  51.640  1.00 23.36      C
ATOM   458  OG1 THR A  77     42.715  19.650  51.672  1.00 23.52      O
ATOM   459  CG2 THR A  77     43.604  17.737  52.851  1.00 23.84      C
ATOM   460  C   THR A  77     43.673  16.285  50.305  1.00 23.65      C
ATOM   461  O   THR A  77     44.781  15.784  50.526  1.00 23.58      O
ATOM   462  N   ALA A  78     42.592  15.562  50.024  1.00 23.68      N
ATOM   463  CA  ALA A  78     42.635  14.104  49.973  1.00 24.18      C
ATOM   464  CB  ALA A  78     41.222  13.534  49.835  1.00 24.04      C
ATOM   465  C   ALA A  78     43.505  13.632  48.817  1.00 24.10      C
ATOM   466  O   ALA A  78     44.275  12.683  48.960  1.00 23.96      O
ATOM   467  N   VAL A  79     43.389  14.288  47.667  1.00 23.77      N
ATOM   468  CA  VAL A  79     44.206  13.892  46.533  1.00 24.22      C
ATOM   469  CB  VAL A  79     43.880  14.714  45.264  1.00 23.88      C
ATOM   470  CG1 VAL A  79     44.830  14.320  44.145  1.00 23.31      C
ATOM   471  CG2 VAL A  79     42.434  14.466  44.834  1.00 23.95      C
ATOM   472  C   VAL A  79     45.683  14.086  46.874  1.00 24.69      C
ATOM   473  O   VAL A  79     46.505  13.204  46.612  1.00 24.55      O
ATOM   474  N   GLN A  80     46.005  15.234  47.465  1.00 25.87      N
ATOM   475  CA  GLN A  80     47.381  15.560  47.847  1.00 27.88      C
ATOM   476  CB  GLN A  80     47.449  16.934  48.524  1.00 28.24      C
ATOM   477  CG  GLN A  80     48.853  17.292  49.006  1.00 29.92      C
ATOM   478  CD  GLN A  80     48.950  18.668  49.616  1.00 30.55      C
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Figure 8J

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ATOM   479 OE1 GLN A 80     48.356 18.943 50.662 1.00 32.95      O
ATOM   480 NE2 GLN A 80     49.703 19.546 48.971 1.00 31.00      N
ATOM   481 C   GLN A 80     47.991 14.521 48.781 1.00 29.34      C
ATOM   482 O   GLN A 80     49.211 14.361 48.833 1.00 28.95      O
ATOM   483 N   GLU A 81     47.143 13.824 49.527 1.00 30.79      N
ATOM   484 CA  GLU A 81     47.617 12.799 50.445 1.00 32.53      C
ATOM   485 CB  GLU A 81     46.525 12.443 51.453 1.00 34.55      C
ATOM   486 CG  GLU A 81     46.442 13.408 52.606 1.00 37.85      C
ATOM   487 CD  GLU A 81     47.735 13.457 53.399 1.00 39.61      C
ATOM   488 OE1 GLU A 81     48.230 12.381 53.806 1.00 41.29      O
ATOM   489 OE2 GLU A 81     48.258 14.569 53.618 1.00 41.33      O
ATOM   490 C   GLU A 81     48.035 11.559 49.675 1.00 32.42      C
ATOM   491 O   GLU A 81     48.974 10.865 50.066 1.00 32.74      O
ATOM   492 N   ARG A 82     47.337 11.285 48.578 1.00 31.81      N
ATOM   493 CA  ARG A 82     47.653 10.135 47.743 1.00 31.83      C
ATOM   494 CB  ARG A 82     46.456  9.777 46.852 1.00 32.76      C
ATOM   495 CG  ARG A 82     45.289  9.128 47.600 1.00 34.95      C
ATOM   496 CD  ARG A 82     45.701  7.773 48.180 1.00 36.27      C
ATOM   497 NE  ARG A 82     45.997  6.810 47.120 1.00 38.20      N
ATOM   498 CZ  ARG A 82     45.085  6.042 46.528 1.00 38.36      C
ATOM   499 NH1 ARG A 82     43.815  6.116 46.899 1.00 38.95      N
ATOM   500 NH2 ARG A 82     45.441  5.212 45.554 1.00 38.87      N
ATOM   501 C   ARG A 82     48.879 10.431 46.877 1.00 31.32      C
ATOM   502 O   ARG A 82     49.741  9.568 46.690 1.00 31.21      O
ATOM   503 N   TYR A 83     48.953 11.650 46.351 1.00 30.58      N
ATOM   504 CA  TYR A 83     50.079 12.057 45.510 1.00 30.30      C
ATOM   505 CB  TYR A 83     49.798 11.802 44.021 1.00 30.71      C
ATOM   506 CG  TYR A 83     49.710 10.362 43.580 1.00 31.39      C
ATOM   507 CD1 TYR A 83     48.481  9.717 43.484 1.00 31.23      C
ATOM   508 CE1 TYR A 83     48.394  8.404 43.034 1.00 32.06      C
ATOM   509 CD2 TYR A 83     50.857  9.655 43.218 1.00 31.62      C
ATOM   510 CE2 TYR A 83     50.780  8.342 42.767 1.00 32.08      C
ATOM   511 CZ  TYR A 83     49.550  7.724 42.677 1.00 32.19      C
ATOM   512 OH  TYR A 83     49.471  6.423 42.229 1.00 32.58      O
ATOM   513 C   TYR A 83     50.408 13.538 45.629 1.00 29.65      C
ATOM   514 O   TYR A 83     49.520 14.385 45.519 1.00 29.22      O
ATOM   515 N   PRO A 84     51.685 13.872 45.875 1.00 29.11      N
ATOM   516 CD  PRO A 84     52.799 13.019 46.335 1.00 29.50      C
ATOM   517 CA  PRO A 84     52.034 15.291 45.966 1.00 28.54      C
ATOM   518 CB  PRO A 84     53.539 15.257 46.206 1.00 29.05      C
ATOM   519 CG  PRO A 84     53.700 14.012 47.048 1.00 29.74      C
ATOM   520 C   PRO A 84     51.681 15.839 44.579 1.00 27.78      C
ATOM   521 O   PRO A 84     51.882 15.156 43.576 1.00 27.15      O
ATOM   522 N   LEU A 85     51.151 17.053 44.518 1.00 27.35      N
ATOM   523 CA  LEU A 85     50.741 17.626 43.239 1.00 26.90      C
ATOM   524 CB  LEU A 85     49.323 18.192 43.361 1.00 26.62      C
ATOM   525 CG  LEU A 85     48.230 17.259 43.889 1.00 26.34      C
ATOM   526 CD1 LEU A 85     46.923 18.030 44.073 1.00 26.18      C
ATOM   527 CD2 LEU A 85     48.049 16.102 42.926 1.00 26.09      C
ATOM   528 C   LEU A 85     51.661 18.725 42.731 1.00 26.93      C
ATOM   529 O   LEU A 85     52.148 19.540 43.501 1.00 26.47      O
ATOM   530 N   ALA A 86     51.908 18.731 41.428 1.00 27.16      N
ATOM   531 CA  ALA A 86     52.727 19.772 40.828 1.00 27.51      C
ATOM   532 CB  ALA A 86     53.411 19.244 39.560 1.00 27.79      C
ATOM   533 C   ALA A 86     51.775 20.922 40.484 1.00 27.57      C
ATOM   534 O   ALA A 86     52.149 22.091 40.512 1.00 28.41      O
ATOM   535 N   LEU A 87     50.524 20.581 40.189 1.00 27.71      N
ATOM   536 CA  LEU A 87     49.530 21.582 39.824 1.00 27.37      C
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Figure 8K

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ATOM   537 CB  LEU A  87     49.866  22.133  38.430  1.00 28.02      C
ATOM   538 CG  LEU A  87     48.916  23.067  37.676  1.00 27.98      C
ATOM   539 CD1 LEU A  87     49.721  23.825  36.624  1.00 28.10      C
ATOM   540 CD2 LEU A  87     47.788  22.274  37.013  1.00 28.31      C
ATOM   541 C   LEU A  87     48.134  20.972  39.817  1.00 27.07      C
ATOM   542 O   LEU A  87     47.973  19.779  39.558  1.00 27.09      O
ATOM   543 N   ALA A  88     47.132  21.797  40.101  1.00 26.70      N
ATOM   544 CA  ALA A  88     45.745  21.353  40.106  1.00 26.24      C
ATOM   545 CB  ALA A  88     45.218  21.285  41.528  1.00 26.54      C
ATOM   546 C   ALA A  88     44.876  22.299  39.282  1.00 26.33      C
ATOM   547 O   ALA A  88     45.040  23.522  39.326  1.00 25.93      O
ATOM   548 N   VAL A  89     43.949  21.719  38.532  1.00 26.38      N
ATOM   549 CA  VAL A  89     43.035  22.493  37.704  1.00 26.48      C
ATOM   550 CB  VAL A  89     43.100  22.057  36.225  1.00 26.98      C
ATOM   551 CG1 VAL A  89     42.184  22.945  35.388  1.00 26.51      C
ATOM   552 CG2 VAL A  89     44.535  22.111  35.719  1.00 26.37      C
ATOM   553 C   VAL A  89     41.605  22.285  38.174  1.00 26.45      C
ATOM   554 O   VAL A  89     41.128  21.153  38.248  1.00 26.61      O
ATOM   555 N   VAL A  90     40.930  23.375  38.513  1.00 26.03      N
ATOM   556 CA  VAL A  90     39.543  23.300  38.928  1.00 26.42      C
ATOM   557 CB  VAL A  90     39.195  24.432  39.916  1.00 26.37      C
ATOM   558 CG1 VAL A  90     37.744  24.315  40.361  1.00 26.82      C
ATOM   559 CG2 VAL A  90     40.123  24.355  41.137  1.00 26.76      C
ATOM   560 C   VAL A  90     38.787  23.490  37.615  1.00 26.74      C
ATOM   561 O   VAL A  90     38.371  24.601  37.288  1.00 26.48      O
ATOM   562 N   ALA A  91     38.657  22.405  36.853  1.00 26.82      N
ATOM   563 CA  ALA A  91     37.986  22.438  35.549  1.00 27.63      C
ATOM   564 CB  ALA A  91     38.468  21.276  34.694  1.00 27.04      C
ATOM   565 C   ALA A  91     36.488  22.356  35.758  1.00 28.11      C
ATOM   566 O   ALA A  91     35.820  21.459  35.242  1.00 27.96      O
ATOM   567 N   CYS A  92     35.979  23.327  36.509  1.00 29.18      N
ATOM   568 CA  CYS A  92     34.579  23.399  36.882  1.00 30.48      C
ATOM   569 CB  CYS A  92     34.402  22.573  38.163  1.00 30.27      C
ATOM   570 SG  CYS A  92     32.819  22.659  38.984  1.00 30.88      S
ATOM   571 C   CYS A  92     34.219  24.867  37.137  1.00 31.39      C
ATOM   572 O   CYS A  92     34.730  25.473  38.075  1.00 31.00      O
ATOM   573 N   ASN A  93     33.341  25.436  36.310  1.00 32.97      N
ATOM   574 CA  ASN A  93     32.937  26.837  36.470  1.00 34.50      C
ATOM   575 CB  ASN A  93     32.043  27.283  35.306  1.00 35.30      C
ATOM   576 CG  ASN A  93     32.770  27.298  33.982  1.00 36.40      C
ATOM   577 OD1 ASN A  93     32.983  26.251  33.360  1.00 37.59      O
ATOM   578 ND2 ASN A  93     33.165  28.489  33.539  1.00 36.95      N
ATOM   579 C   ASN A  93     32.218  27.128  37.784  1.00 35.02      C
ATOM   580 O   ASN A  93     32.473  28.151  38.426  1.00 35.62      O
ATOM   581 N   THR A  94     31.317  26.236  38.183  1.00 35.16      N
ATOM   582 CA  THR A  94     30.567  26.418  39.420  1.00 36.16      C
ATOM   583 CB  THR A  94     29.417  25.389  39.539  1.00 36.42      C
ATOM   584 OG1 THR A  94     29.934  24.063  39.353  1.00 36.99      O
ATOM   585 CG2 THR A  94     28.354  25.662  38.493  1.00 36.28      C
ATOM   586 C   THR A  94     31.436  26.311  40.668  1.00 36.39      C
ATOM   587 O   THR A  94     30.972  26.572  41.774  1.00 37.04      O
ATOM   588 N   ALA A  95     32.695  25.928  40.501  1.00 36.62      N
ATOM   589 CA  ALA A  95     33.587  25.803  41.654  1.00 37.07      C
ATOM   590 CB  ALA A  95     34.093  24.363  41.780  1.00 36.87      C
ATOM   591 C   ALA A  95     34.769  26.757  41.599  1.00 37.26      C
ATOM   592 O   ALA A  95     35.183  27.291  42.626  1.00 37.43      O
ATOM   593 N   SER A  96     35.304  26.978  40.405  1.00 37.85      N
ATOM   594 CA  SER A  96     36.464  27.844  40.245  1.00 38.98      C
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Figure 8L

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ATOM   595  CB  SER A  96      36.701  28.167  38.772  1.00 38.43           C
ATOM   596  OG  SER A  96      37.534  27.193  38.172  1.00 39.50           O
ATOM   597  C   SER A  96      36.403  29.140  41.031  1.00 39.55           C
ATOM   598  O   SER A  96      37.056  29.276  42.064  1.00 40.03           O
ATOM   599  N   THR A  97      35.621  30.090  40.540  1.00 40.03           N
ATOM   600  CA  THR A  97      35.507  31.386  41.193  1.00 40.80           C
ATOM   601  CB  THR A  97      34.206  32.086  40.782  1.00 41.54           C
ATOM   602  OG1 THR A  97      33.079  31.351  41.283  1.00 43.65           O
ATOM   603  CG2 THR A  97      34.116  32.152  39.266  1.00 42.47           C
ATOM   604  C   THR A  97      35.580  31.334  42.718  1.00 40.13           C
ATOM   605  O   THR A  97      36.587  31.730  43.322  1.00 40.25           O
ATOM   606  N   VAL A  98      34.524  30.819  43.333  1.00 38.98           N
ATOM   607  CA  VAL A  98      34.440  30.749  44.783  1.00 37.63           C
ATOM   608  CB  VAL A  98      33.074  30.183  45.210  1.00 38.05           C
ATOM   609  CG1 VAL A  98      31.951  31.032  44.616  1.00 37.94           C
ATOM   610  CG2 VAL A  98      32.949  28.735  44.752  1.00 37.58           C
ATOM   611  C   VAL A  98      35.521  29.956  45.520  1.00 36.84           C
ATOM   612  O   VAL A  98      35.789  30.230  46.689  1.00 36.41           O
ATOM   613  N   SER A  99      36.145  28.989  44.848  1.00 35.65           N
ATOM   614  CA  SER A  99      37.149  28.136  45.491  1.00 34.62           C
ATOM   615  CB  SER A  99      36.982  26.688  45.001  1.00 34.67           C
ATOM   616  OG  SER A  99      35.697  26.177  45.311  1.00 35.45           O
ATOM   617  C   SER A  99      38.626  28.504  45.353  1.00 33.65           C
ATOM   618  O   SER A  99      39.443  28.075  46.165  1.00 33.61           O
ATOM   619  N   LEU A 100      38.974  29.278  44.335  1.00 32.41           N
ATOM   620  CA  LEU A 100      40.371  29.635  44.103  1.00 31.86           C
ATOM   621  CB  LEU A 100      40.476  30.501  42.844  1.00 31.39           C
ATOM   622  CG  LEU A 100      40.052  29.816  41.538  1.00 31.77           C
ATOM   623  CD1 LEU A 100      40.345  30.741  40.359  1.00 31.20           C
ATOM   624  CD2 LEU A 100      40.813  28.498  41.363  1.00 31.65           C
ATOM   625  C   LEU A 100      41.131  30.286  45.272  1.00 31.53           C
ATOM   626  O   LEU A 100      42.227  29.851  45.620  1.00 31.21           O
ATOM   627  N   PRO A 101      40.570  31.336  45.887  1.00 31.41           N
ATOM   628  CD  PRO A 101      39.378  32.122  45.526  1.00 31.74           C
ATOM   629  CA  PRO A 101      41.289  31.958  47.006  1.00 31.39           C
ATOM   630  CB  PRO A 101      40.312  33.027  47.488  1.00 31.54           C
ATOM   631  CG  PRO A 101      39.657  33.455  46.202  1.00 31.94           C
ATOM   632  C   PRO A 101      41.642  30.960  48.111  1.00 31.01           C
ATOM   633  O   PRO A 101      42.784  30.908  48.574  1.00 30.97           O
ATOM   634  N   ALA A 102      40.657  30.168  48.522  1.00 30.66           N
ATOM   635  CA  ALA A 102      40.845  29.180  49.579  1.00 30.28           C
ATOM   636  CB  ALA A 102      39.507  28.531  49.927  1.00 30.65           C
ATOM   637  C   ALA A 102      41.867  28.110  49.210  1.00 29.99           C
ATOM   638  O   ALA A 102      42.675  27.692  50.049  1.00 29.77           O
ATOM   639  N   LEU A 103      41.833  27.668  47.957  1.00 29.36           N
ATOM   640  CA  LEU A 103      42.764  26.650  47.483  1.00 28.42           C
ATOM   641  CB  LEU A 103      42.322  26.126  46.119  1.00 27.97           C
ATOM   642  CG  LEU A 103      41.031  25.302  46.119  1.00 27.49           C
ATOM   643  CD1 LEU A 103      40.535  25.118  44.684  1.00 26.76           C
ATOM   644  CD2 LEU A 103      41.286  23.957  46.790  1.00 26.64           C
ATOM   645  C   LEU A 103      44.184  27.189  47.378  1.00 28.66           C
ATOM   646  O   LEU A 103      45.145  26.503  47.722  1.00 27.90           O
ATOM   647  N   ARG A 104      44.315  28.424  46.911  1.00 28.64           N
ATOM   648  CA  ARG A 104      45.630  29.021  46.761  1.00 29.38           C
ATOM   649  CB  ARG A 104      45.540  30.265  45.875  1.00 29.44           C
ATOM   650  CG  ARG A 104      45.362  29.904  44.407  1.00 30.55           C
ATOM   651  CD  ARG A 104      44.967  31.091  43.526  1.00 31.09           C
ATOM   652  NE  ARG A 104      44.866  30.655  42.134  1.00 31.83           N
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Figure 8M

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ATOM   653  CZ  ARG A 104      44.212  31.307  41.175  1.00 31.39           C
ATOM   654  NH1 ARG A 104      43.585  32.442  41.439  1.00 31.47           N
ATOM   655  NH2 ARG A 104      44.180  30.810  39.950  1.00 30.99           N
ATOM   656  C   ARG A 104      46.261  29.346  48.104  1.00 29.24           C
ATOM   657  O   ARG A 104      47.477  29.439  48.213  1.00 28.87           O
ATOM   658  N   GLU A 105      45.430  29.507  49.126  1.00 29.80           N
ATOM   659  CA  GLU A 105      45.928  29.791  50.465  1.00 31.03           C
ATOM   660  CB  GLU A 105      44.831  30.424  51.328  1.00 32.41           C
ATOM   661  CG  GLU A 105      45.138  30.405  52.827  1.00 34.95           C
ATOM   662  CD  GLU A 105      46.373  31.213  53.190  1.00 36.39           C
ATOM   663  OE1 GLU A 105      46.929  30.992  54.294  1.00 37.63           O
ATOM   664  OE2 GLU A 105      46.785  32.072  52.379  1.00 37.49           O
ATOM   665  C   GLU A 105      46.408  28.503  51.129  1.00 30.44           C
ATOM   666  O   GLU A 105      47.463  28.476  51.761  1.00 31.06           O
ATOM   667  N   LYS A 106      45.648  27.428  50.972  1.00 29.73           N
ATOM   668  CA  LYS A 106      46.023  26.175  51.605  1.00 29.26           C
ATOM   669  CB  LYS A 106      44.806  25.245  51.723  1.00 29.20           C
ATOM   670  CG  LYS A 106      45.091  24.005  52.595  1.00 29.25           C
ATOM   671  CD  LYS A 106      43.840  23.174  52.882  1.00 28.92           C
ATOM   672  CE  LYS A 106      44.150  22.010  53.840  1.00 28.67           C
ATOM   673  NZ  LYS A 106      42.965  21.124  54.082  1.00 28.66           N
ATOM   674  C   LYS A 106      47.168  25.410  50.943  1.00 29.05           C
ATOM   675  O   LYS A 106      47.993  24.806  51.635  1.00 28.51           O
ATOM   676  N   PHE A 107      47.240  25.445  49.617  1.00 28.37           N
ATOM   677  CA  PHE A 107      48.270  24.690  48.925  1.00 28.51           C
ATOM   678  CB  PHE A 107      47.627  23.857  47.815  1.00 28.11           C
ATOM   679  CG  PHE A 107      46.516  22.973  48.308  1.00 27.86           C
ATOM   680  CD1 PHE A 107      45.185  23.346  48.147  1.00 27.53           C
ATOM   681  CD2 PHE A 107      46.805  21.795  48.991  1.00 27.75           C
ATOM   682  CE1 PHE A 107      44.156  22.560  48.665  1.00 27.08           C
ATOM   683  CE2 PHE A 107      45.781  20.997  49.514  1.00 27.41           C
ATOM   684  CZ  PHE A 107      44.457  21.383  49.350  1.00 27.01           C
ATOM   685  C   PHE A 107      49.443  25.476  48.376  1.00 28.85           C
ATOM   686  O   PHE A 107      49.337  26.669  48.096  1.00 28.61           O
ATOM   687  N   ASP A 108      50.566  24.781  48.225  1.00 29.16           N
ATOM   688  CA  ASP A 108      51.781  25.394  47.716  1.00 29.72           C
ATOM   689  CB  ASP A 108      52.925  25.180  48.700  1.00 29.47           C
ATOM   690  CG  ASP A 108      52.721  25.959  49.973  1.00 29.74           C
ATOM   691  OD1 ASP A 108      52.567  27.196  49.880  1.00 29.19           O
ATOM   692  OD2 ASP A 108      52.700  25.344  51.058  1.00 29.72           O
ATOM   693  C   ASP A 108      52.163  24.914  46.333  1.00 29.83           C
ATOM   694  O   ASP A 108      53.335  24.699  46.018  1.00 30.36           O
ATOM   695  N   PHE A 109      51.145  24.724  45.511  1.00 29.48           N
ATOM   696  CA  PHE A 109      51.345  24.342  44.128  1.00 29.36           C
ATOM   697  CB  PHE A 109      51.079  22.844  43.895  1.00 28.81           C
ATOM   698  CG  PHE A 109      49.781  22.348  44.454  1.00 29.18           C
ATOM   699  CD1 PHE A 109      48.568  22.679  43.851  1.00 29.09           C
ATOM   700  CD2 PHE A 109      49.772  21.525  45.579  1.00 28.19           C
ATOM   701  CE1 PHE A 109      47.363  22.194  44.364  1.00 29.20           C
ATOM   702  CE2 PHE A 109      48.580  21.037  46.099  1.00 28.87           C
ATOM   703  CZ  PHE A 109      47.368  21.369  45.492  1.00 28.19           C
ATOM   704  C   PHE A 109      50.358  25.232  43.397  1.00 28.99           C
ATOM   705  O   PHE A 109      49.331  25.626  43.956  1.00 28.79           O
ATOM   706  N   PRO A 110      50.673  25.600  42.153  1.00 29.04           N
ATOM   707  CD  PRO A 110      51.823  25.213  41.318  1.00 28.89           C
ATOM   708  CA  PRO A 110      49.751  26.467  41.419  1.00 29.02           C
ATOM   709  CB  PRO A 110      50.515  26.761  40.128  1.00 28.79           C
ATOM   710  CG  PRO A 110      51.326  25.525  39.929  1.00 29.59           C
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Figure 8N

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ATOM   711  C   PRO A 110     48.381  25.839  41.182  1.00 28.61           C
ATOM   712  O   PRO A 110     48.259  24.630  40.990  1.00 28.77           O
ATOM   713  N   VAL A 111     47.352  26.673  41.224  1.00 28.61           N
ATOM   714  CA  VAL A 111     45.989  26.215  41.002  1.00 28.17           C
ATOM   715  CB  VAL A 111     45.101  26.457  42.240  1.00 27.94           C
ATOM   716  CG1 VAL A 111     43.683  25.945  41.978  1.00 26.91           C
ATOM   717  CG2 VAL A 111     45.710  25.759  43.467  1.00 27.23           C
ATOM   718  C   VAL A 111     45.417  26.987  39.822  1.00 28.51           C
ATOM   719  O   VAL A 111     45.482  28.213  39.786  1.00 28.55           O
ATOM   720  N   VAL A 112     44.871  26.263  38.854  1.00 28.78           N
ATOM   721  CA  VAL A 112     44.284  26.892  37.679  1.00 29.08           C
ATOM   722  CB  VAL A 112     44.691  26.145  36.387  1.00 29.31           C
ATOM   723  CG1 VAL A 112     43.996  26.753  35.175  1.00 29.34           C
ATOM   724  CG2 VAL A 112     46.185  26.215  36.213  1.00 28.86           C
ATOM   725  C   VAL A 112     42.772  26.891  37.810  1.00 29.49           C
ATOM   726  O   VAL A 112     42.175  25.895  38.227  1.00 29.47           O
ATOM   727  N   GLY A 113     42.160  28.021  37.475  1.00 29.33           N
ATOM   728  CA  GLY A 113     40.719  28.132  37.551  1.00 29.94           C
ATOM   729  C   GLY A 113     40.136  28.309  36.164  1.00 30.66           C
ATOM   730  O   GLY A 113     40.873  28.407  35.180  1.00 29.81           O
ATOM   731  N   VAL A 114     38.809  28.351  36.088  1.00 31.45           N
ATOM   732  CA  VAL A 114     38.121  28.518  34.811  1.00 32.36           C
ATOM   733  CB  VAL A 114     37.509  27.204  34.315  1.00 32.77           C
ATOM   734  CG1 VAL A 114     38.587  26.138  34.165  1.00 32.86           C
ATOM   735  CG2 VAL A 114     36.425  26.756  35.276  1.00 33.24           C
ATOM   736  C   VAL A 114     36.983  29.521  34.894  1.00 32.64           C
ATOM   737  O   VAL A 114     36.178  29.505  35.833  1.00 33.94           O
ATOM   738  N   VAL A 115     36.932  30.409  33.913  1.00 31.91           N
ATOM   739  CA  VAL A 115     35.869  31.395  33.830  1.00 31.47           C
ATOM   740  CB  VAL A 115     36.368  32.820  34.173  1.00 32.15           C
ATOM   741  CG1 VAL A 115     36.717  32.908  35.652  1.00 33.28           C
ATOM   742  CG2 VAL A 115     37.579  33.169  33.330  1.00 32.44           C
ATOM   743  C   VAL A 115     35.409  31.348  32.375  1.00 30.19           C
ATOM   744  O   VAL A 115     36.202  31.048  31.483  1.00 29.34           O
ATOM   745  N   PRO A 116     34.122  31.615  32.121  1.00 29.68           N
ATOM   746  CD  PRO A 116     33.044  31.894  33.088  1.00 29.83           C
ATOM   747  CA  PRO A 116     33.610  31.590  30.743  1.00 28.99           C
ATOM   748  CB  PRO A 116     32.195  32.141  30.894  1.00 29.53           C
ATOM   749  CG  PRO A 116     31.793  31.619  32.267  1.00 29.52           C
ATOM   750  C   PRO A 116     34.482  32.445  29.826  1.00 28.73           C
ATOM   751  O   PRO A 116     34.865  33.560  30.194  1.00 28.39           O
ATOM   752  N   ALA A 117     34.786  31.921  28.639  1.00 27.82           N
ATOM   753  CA  ALA A 117     35.638  32.607  27.663  1.00 28.21           C
ATOM   754  CB  ALA A 117     36.125  31.607  26.614  1.00 26.94           C
ATOM   755  C   ALA A 117     34.977  33.800  26.974  1.00 28.60           C
ATOM   756  O   ALA A 117     35.023  33.930  25.747  1.00 28.59           O
ATOM   757  N   ILE A 118     34.376  34.676  27.766  1.00 28.96           N
ATOM   758  CA  ILE A 118     33.710  35.848  27.225  1.00 29.91           C
ATOM   759  CB  ILE A 118     32.962  36.606  28.335  1.00 31.06           C
ATOM   760  CG2 ILE A 118     32.449  37.950  27.808  1.00 31.44           C
ATOM   761  CG1 ILE A 118     31.809  35.736  28.844  1.00 31.63           C
ATOM   762  CD1 ILE A 118     31.091  36.303  30.038  1.00 33.47           C
ATOM   763  C   ILE A 118     34.673  36.800  26.537  1.00 30.04           C
ATOM   764  O   ILE A 118     34.367  37.329  25.466  1.00 29.91           O
ATOM   765  N   LYS A 119     35.840  37.008  27.143  1.00 29.81           N
ATOM   766  CA  LYS A 119     36.836  37.915  26.584  1.00 30.04           C
ATOM   767  CB  LYS A 119     38.091  37.933  27.468  1.00 30.22           C
ATOM   768  CG  LYS A 119     39.130  38.955  27.020  1.00 30.96           C
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Figure 8O

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ATOM   769  CD  LYS A 119      40.292  39.050  27.988  1.00 31.45           C
ATOM   770  CE  LYS A 119      41.314  40.048  27.492  1.00 31.36           C
ATOM   771  NZ  LYS A 119      42.566  39.971  28.280  1.00 32.08           N
ATOM   772  C   LYS A 119      37.210  37.606  25.125  1.00 30.26           C
ATOM   773  O   LYS A 119      37.081  38.468  24.260  1.00 30.43           O
ATOM   774  N   PRO A 120      37.687  36.385  24.829  1.00 30.32           N
ATOM   775  CD  PRO A 120      38.119  35.261  25.679  1.00 30.42           C
ATOM   776  CA  PRO A 120      38.024  36.135  23.424  1.00 30.77           C
ATOM   777  CB  PRO A 120      38.743  34.782  23.469  1.00 30.78           C
ATOM   778  CG  PRO A 120      38.175  34.123  24.687  1.00 30.65           C
ATOM   779  C   PRO A 120      36.805  36.124  22.501  1.00 31.13           C
ATOM   780  O   PRO A 120      36.900  36.515  21.339  1.00 31.33           O
ATOM   781  N   ALA A 121      35.662  35.684  23.018  1.00 31.38           N
ATOM   782  CA  ALA A 121      34.447  35.632  22.214  1.00 31.88           C
ATOM   783  CB  ALA A 121      33.317  35.001  23.007  1.00 31.22           C
ATOM   784  C   ALA A 121      34.049  37.030  21.754  1.00 32.64           C
ATOM   785  O   ALA A 121      33.558  37.206  20.637  1.00 32.09           O
ATOM   786  N   ALA A 122      34.268  38.019  22.618  1.00 33.55           N
ATOM   787  CA  ALA A 122      33.931  39.405  22.305  1.00 34.91           C
ATOM   788  CB  ALA A 122      34.108  40.281  23.544  1.00 34.63           C
ATOM   789  C   ALA A 122      34.779  39.944  21.159  1.00 35.90           C
ATOM   790  O   ALA A 122      34.334  40.809  20.408  1.00 36.06           O
ATOM   791  N   ARG A 123      36.000  39.435  21.029  1.00 37.08           N
ATOM   792  CA  ARG A 123      36.901  39.866  19.962  1.00 38.64           C
ATOM   793  CB  ARG A 123      38.363  39.696  20.382  1.00 39.68           C
ATOM   794  CG  ARG A 123      38.775  40.468  21.618  1.00 41.76           C
ATOM   795  CD  ARG A 123      40.279  40.379  21.811  1.00 43.75           C
ATOM   796  NE  ARG A 123      41.000  40.999  20.701  1.00 45.71           N
ATOM   797  CZ  ARG A 123      42.320  40.959  20.547  1.00 46.46           C
ATOM   798  NH1 ARG A 123      43.071  40.321  21.435  1.00 47.45           N
ATOM   799  NH2 ARG A 123      42.891  41.564  19.512  1.00 47.03           N
ATOM   800  C   ARG A 123      36.689  39.068  18.678  1.00 39.10           C
ATOM   801  O   ARG A 123      37.252  39.405  17.636  1.00 39.34           O
ATOM   802  N   LEU A 124      35.886  38.011  18.749  1.00 39.13           N
ATOM   803  CA  LEU A 124      35.653  37.165  17.583  1.00 39.56           C
ATOM   804  CB  LEU A 124      35.776  35.686  17.975  1.00 39.49           C
ATOM   805  CG  LEU A 124      37.133  35.224  18.517  1.00 39.90           C
ATOM   806  CD1 LEU A 124      37.039  33.765  18.952  1.00 40.24           C
ATOM   807  CD2 LEU A 124      38.210  35.398  17.455  1.00 40.03           C
ATOM   808  C   LEU A 124      34.315  37.391  16.895  1.00 39.81           C
ATOM   809  O   LEU A 124      34.197  37.192  15.685  1.00 39.83           O
ATOM   810  N   THR A 125      33.311  37.807  17.659  1.00 39.86           N
ATOM   811  CA  THR A 125      31.991  38.027  17.096  1.00 40.44           C
ATOM   812  CB  THR A 125      30.981  38.482  18.179  1.00 40.32           C
ATOM   813  OG1 THR A 125      29.685  38.636  17.589  1.00 40.44           O
ATOM   814  CG2 THR A 125      31.411  39.803  18.809  1.00 40.44           C
ATOM   815  C   THR A 125      32.023  39.057  15.971  1.00 41.06           C
ATOM   816  O   THR A 125      32.777  40.028  16.022  1.00 40.79           O
ATOM   817  N   ALA A 126      31.206  38.826  14.949  1.00 41.50           N
ATOM   818  CA  ALA A 126      31.133  39.732  13.812  1.00 42.01           C
ATOM   819  CB  ALA A 126      31.214  38.943  12.507  1.00 41.90           C
ATOM   820  C   ALA A 126      29.837  40.532  13.861  1.00 42.35           C
ATOM   821  O   ALA A 126      29.798  41.685  13.427  1.00 42.99           O
ATOM   822  N   ASN A 127      28.778  39.928  14.394  1.00 41.88           N
ATOM   823  CA  ASN A 127      27.493  40.613  14.476  1.00 41.62           C
ATOM   824  CB  ASN A 127      26.350  39.641  14.147  1.00 41.84           C
ATOM   825  CG  ASN A 127      26.027  38.692  15.291  1.00 41.92           C
ATOM   826  OD1 ASN A 127      26.847  38.451  16.175  1.00 41.99           O
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Figure 8P

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ATOM   827 ND2 ASN A 127     24.822  38.135  15.264  1.00 41.74      N
ATOM   828 C   ASN A 127     27.266  41.262  15.834  1.00 41.10      C
ATOM   829 O   ASN A 127     26.241  41.902  16.066  1.00 41.43      O
ATOM   830 N   GLY A 128     28.234  41.101  16.730  1.00 40.81      N
ATOM   831 CA  GLY A 128     28.122  41.688  18.052  1.00 39.82      C
ATOM   832 C   GLY A 128     27.185  40.965  19.004  1.00 39.18      C
ATOM   833 O   GLY A 128     26.933  41.453  20.103  1.00 39.41      O
ATOM   834 N   ILE A 129     26.660  39.812  18.594  1.00 38.60      N
ATOM   835 CA  ILE A 129     25.757  39.044  19.451  1.00 37.56      C
ATOM   836 CB  ILE A 129     24.523  38.522  18.686  1.00 37.63      C
ATOM   837 CG2 ILE A 129     23.450  38.100  19.686  1.00 37.28      C
ATOM   838 CG1 ILE A 129     23.980  39.593  17.732  1.00 38.02      C
ATOM   839 CD1 ILE A 129     23.250  40.727  18.406  1.00 38.18      C
ATOM   840 C   ILE A 129     26.510  37.822  19.983  1.00 36.88      C
ATOM   841 O   ILE A 129     26.787  36.882  19.241  1.00 36.65      O
ATOM   842 N   VAL A 130     26.834  37.840  21.270  1.00 35.90      N
ATOM   843 CA  VAL A 130     27.554  36.733  21.877  1.00 34.41      C
ATOM   844 CB  VAL A 130     28.823  37.233  22.594  1.00 34.44      C
ATOM   845 CG1 VAL A 130     29.512  36.079  23.314  1.00 34.63      C
ATOM   846 CG2 VAL A 130     29.768  37.857  21.578  1.00 33.95      C
ATOM   847 C   VAL A 130     26.674  35.990  22.870  1.00 33.52      C
ATOM   848 O   VAL A 130     26.082  36.589  23.770  1.00 33.77      O
ATOM   849 N   GLY A 131     26.583  34.679  22.695  1.00 32.38      N
ATOM   850 CA  GLY A 131     25.779  33.877  23.593  1.00 31.20      C
ATOM   851 C   GLY A 131     26.626  33.212  24.667  1.00 30.54      C
ATOM   852 O   GLY A 131     27.799  32.903  24.453  1.00 29.56      O
ATOM   853 N   LEU A 132     26.032  33.009  25.837  1.00 29.94      N
ATOM   854 CA  LEU A 132     26.726  32.348  26.930  1.00 29.63      C
ATOM   855 CB  LEU A 132     26.970  33.314  28.094  1.00 29.35      C
ATOM   856 CG  LEU A 132     27.559  32.707  29.383  1.00 29.67      C
ATOM   857 CD1 LEU A 132     28.930  32.091  29.115  1.00 28.73      C
ATOM   858 CD2 LEU A 132     27.676  33.800  30.444  1.00 29.83      C
ATOM   859 C   LEU A 132     25.870  31.189  27.402  1.00 29.56      C
ATOM   860 O   LEU A 132     24.764  31.392  27.912  1.00 29.35      O
ATOM   861 N   LEU A 133     26.362  29.975  27.190  1.00 29.49      N
ATOM   862 CA  LEU A 133     25.658  28.776  27.632  1.00 30.26      C
ATOM   863 CB  LEU A 133     25.747  27.655  26.596  1.00 29.82      C
ATOM   864 CG  LEU A 133     24.832  27.685  25.382  1.00 29.97      C
ATOM   865 CD1 LEU A 133     25.087  26.431  24.561  1.00 29.36      C
ATOM   866 CD2 LEU A 133     23.370  27.738  25.831  1.00 29.56      C
ATOM   867 C   LEU A 133     26.374  28.328  28.891  1.00 30.96      C
ATOM   868 O   LEU A 133     27.577  28.064  28.867  1.00 30.93      O
ATOM   869 N   ALA A 134     25.641  28.258  29.991  1.00 31.95      N
ATOM   870 CA  ALA A 134     26.220  27.838  31.256  1.00 33.61      C
ATOM   871 CB  ALA A 134     26.671  29.056  32.057  1.00 33.35      C
ATOM   872 C   ALA A 134     25.157  27.080  32.022  1.00 34.73      C
ATOM   873 O   ALA A 134     24.021  26.963  31.567  1.00 34.36      O
ATOM   874 N   THR A 135     25.515  26.552  33.184  1.00 36.55      N
ATOM   875 CA  THR A 135     24.522  25.845  33.960  1.00 38.50      C
ATOM   876 CB  THR A 135     25.166  24.865  34.958  1.00 38.44      C
ATOM   877 OG1 THR A 135     24.136  24.057  35.544  1.00 38.63      O
ATOM   878 CG2 THR A 135     25.932  25.610  36.037  1.00 37.99      C
ATOM   879 C   THR A 135     23.676  26.890  34.683  1.00 40.21      C
ATOM   880 O   THR A 135     24.069  28.056  34.790  1.00 39.88      O
ATOM   881 N   ARG A 136     22.514  26.470  35.169  1.00 42.42      N
ATOM   882 CA  ARG A 136     21.592  27.374  35.840  1.00 44.95      C
ATOM   883 CB  ARG A 136     20.419  26.584  36.429  1.00 44.96      C
ATOM   884 CG  ARG A 136     19.310  27.468  36.958  1.00 45.04      C
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Figure 8Q

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ATOM   885  CD  ARG A 136      18.840  28.437  35.880  1.00 44.89           C
ATOM   886  NE  ARG A 136      18.043  29.521  36.442  1.00 45.05           N
ATOM   887  CZ  ARG A 136      17.561  30.538  35.736  1.00 44.74           C
ATOM   888  NH1 ARG A 136      17.794  30.611  34.433  1.00 44.68           N
ATOM   889  NH2 ARG A 136      16.854  31.484  36.337  1.00 44.28           N
ATOM   890  C   ARG A 136      22.226  28.242  36.921  1.00 46.64           C
ATOM   891  O   ARG A 136      21.963  29.443  36.987  1.00 46.85           O
ATOM   892  N   GLY A 137      23.064  27.637  37.759  1.00 48.47           N
ATOM   893  CA  GLY A 137      23.705  28.383  38.828  1.00 50.63           C
ATOM   894  C   GLY A 137      24.761  29.390  38.405  1.00 52.15           C
ATOM   895  O   GLY A 137      24.957  30.403  39.077  1.00 52.40           O
ATOM   896  N   THR A 138      25.439  29.122  37.295  1.00 53.81           N
ATOM   897  CA  THR A 138      26.493  30.007  36.804  1.00 55.54           C
ATOM   898  CB  THR A 138      27.342  29.297  35.732  1.00 55.54           C
ATOM   899  OG1 THR A 138      27.916  28.110  36.292  1.00 55.73           O
ATOM   900  CG2 THR A 138      28.458  30.209  35.236  1.00 55.51           C
ATOM   901  C   THR A 138      25.984  31.326  36.223  1.00 56.87           C
ATOM   902  O   THR A 138      26.685  32.337  36.264  1.00 57.03           O
ATOM   903  N   VAL A 139      24.769  31.314  35.682  1.00 58.47           N
ATOM   904  CA  VAL A 139      24.190  32.516  35.087  1.00 60.06           C
ATOM   905  CB  VAL A 139      23.136  32.151  34.009  1.00 59.85           C
ATOM   906  CG1 VAL A 139      23.805  31.438  32.846  1.00 59.91           C
ATOM   907  CG2 VAL A 139      22.055  31.273  34.613  1.00 59.77           C
ATOM   908  C   VAL A 139      23.537  33.432  36.123  1.00 61.27           C
ATOM   909  O   VAL A 139      23.011  34.495  35.783  1.00 61.39           O
ATOM   910  N   LYS A 140      23.581  33.020  37.386  1.00 62.64           N
ATOM   911  CA  LYS A 140      22.987  33.797  38.471  1.00 64.06           C
ATOM   912  CB  LYS A 140      22.045  32.902  39.285  1.00 64.35           C
ATOM   913  CG  LYS A 140      21.287  33.610  40.403  1.00 64.87           C
ATOM   914  CD  LYS A 140      20.275  32.679  41.073  1.00 65.20           C
ATOM   915  CE  LYS A 140      20.948  31.483  41.739  1.00 65.27           C
ATOM   916  NZ  LYS A 140      21.879  31.897  42.826  1.00 65.54           N
ATOM   917  C   LYS A 140      24.071  34.378  39.379  1.00 64.96           C
ATOM   918  O   LYS A 140      23.778  35.104  40.331  1.00 65.26           O
ATOM   919  N   ARG A 141      25.323  34.057  39.070  1.00 65.90           N
ATOM   920  CA  ARG A 141      26.464  34.523  39.850  1.00 66.86           C
ATOM   921  CB  ARG A 141      27.653  33.584  39.639  1.00 67.34           C
ATOM   922  CG  ARG A 141      27.501  32.230  40.306  1.00 68.13           C
ATOM   923  CD  ARG A 141      27.641  32.357  41.813  1.00 68.85           C
ATOM   924  NE  ARG A 141      27.467  31.079  42.497  1.00 69.48           N
ATOM   925  CZ  ARG A 141      26.332  30.387  42.510  1.00 69.74           C
ATOM   926  NH1 ARG A 141      25.263  30.847  41.873  1.00 69.96           N
ATOM   927  NH2 ARG A 141      26.262  29.238  43.167  1.00 69.94           N
ATOM   928  C   ARG A 141      26.889  35.946  39.511  1.00 67.23           C
ATOM   929  O   ARG A 141      26.868  36.353  38.349  1.00 67.16           O
ATOM   930  N   SER A 142      27.283  36.695  40.537  1.00 67.70           N
ATOM   931  CA  SER A 142      27.733  38.069  40.354  1.00 68.23           C
ATOM   932  CB  SER A 142      27.953  38.742  41.713  1.00 68.35           C
ATOM   933  OG  SER A 142      28.985  38.101  42.441  1.00 68.33           O
ATOM   934  C   SER A 142      29.040  38.061  39.567  1.00 68.56           C
ATOM   935  O   SER A 142      29.280  38.931  38.731  1.00 68.56           O
ATOM   936  N   TYR A 143      29.878  37.067  39.845  1.00 68.92           N
ATOM   937  CA  TYR A 143      31.164  36.921  39.171  1.00 69.28           C
ATOM   938  CB  TYR A 143      31.829  35.609  39.605  1.00 69.43           C
ATOM   939  CG  TYR A 143      33.270  35.440  39.157  1.00 69.75           C
ATOM   940  CD1 TYR A 143      33.605  35.365  37.804  1.00 69.92           C
ATOM   941  CE1 TYR A 143      34.930  35.193  37.395  1.00 69.93           C
ATOM   942  CD2 TYR A 143      34.300  35.339  40.094  1.00 69.94           C
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Figure 8R

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ATOM   943  CE2 TYR A 143     35.628  35.165  39.697  1.00 69.89       C
ATOM   944  CZ  TYR A 143     35.935  35.093  38.346  1.00 69.96       C
ATOM   945  OH  TYR A 143     37.243  34.918  37.950  1.00 69.93       O
ATOM   946  C   TYR A 143     30.945  36.916  37.659  1.00 69.53       C
ATOM   947  O   TYR A 143     31.741  37.474  36.900  1.00 69.51       O
ATOM   948  N   THR A 144     29.857  36.286  37.229  1.00 69.65       N
ATOM   949  CA  THR A 144     29.539  36.207  35.811  1.00 70.00       C
ATOM   950  CB  THR A 144     28.400  35.200  35.553  1.00 69.84       C
ATOM   951  OG1 THR A 144     28.718  33.944  36.168  1.00 69.88       O
ATOM   952  CG2 THR A 144     28.210  34.987  34.056  1.00 69.88       C
ATOM   953  C   THR A 144     29.123  37.577  35.277  1.00 70.22       C
ATOM   954  O   THR A 144     29.803  38.149  34.424  1.00 70.09       O
ATOM   955  N   HIS A 145     28.011  38.096  35.794  1.00 70.56       N
ATOM   956  CA  HIS A 145     27.484  39.395  35.378  1.00 70.96       C
ATOM   957  CB  HIS A 145     26.435  39.893  36.380  1.00 71.08       C
ATOM   958  CG  HIS A 145     25.333  38.916  36.643  1.00 71.36       C
ATOM   959  CD2 HIS A 145     24.826  38.435  37.803  1.00 71.32       C
ATOM   960  ND1 HIS A 145     24.602  38.327  35.633  1.00 71.38       N
ATOM   961  CE1 HIS A 145     23.694  37.525  36.160  1.00 71.57       C
ATOM   962  NE2 HIS A 145     23.809  37.572  37.475  1.00 71.52       N
ATOM   963  C   HIS A 145     28.582  40.446  35.245  1.00 71.08       C
ATOM   964  O   HIS A 145     28.543  41.296  34.354  1.00 71.07       O
ATOM   965  N   GLU A 146     29.559  40.381  36.142  1.00 71.21       N
ATOM   966  CA  GLU A 146     30.671  41.321  36.139  1.00 71.44       C
ATOM   967  CB  GLU A 146     31.480  41.165  37.428  1.00 71.84       C
ATOM   968  CG  GLU A 146     30.672  41.443  38.688  1.00 72.39       C
ATOM   969  CD  GLU A 146     31.393  41.024  39.956  1.00 72.71       C
ATOM   970  OE1 GLU A 146     30.792  41.143  41.043  1.00 73.01       O
ATOM   971  OE2 GLU A 146     32.558  40.576  39.868  1.00 72.85       O
ATOM   972  C   GLU A 146     31.575  41.116  34.930  1.00 71.35       C
ATOM   973  O   GLU A 146     31.878  42.063  34.206  1.00 71.49       O
ATOM   974  N   LEU A 147     32.004  39.876  34.714  1.00 71.27       N
ATOM   975  CA  LEU A 147     32.874  39.556  33.589  1.00 71.04       C
ATOM   976  CB  LEU A 147     33.146  38.050  33.546  1.00 71.09       C
ATOM   977  CG  LEU A 147     34.138  37.538  32.498  1.00 71.03       C
ATOM   978  CD1 LEU A 147     35.511  38.141  32.744  1.00 70.98       C
ATOM   979  CD2 LEU A 147     34.213  36.021  32.574  1.00 71.22       C
ATOM   980  C   LEU A 147     32.232  40.000  32.277  1.00 70.90       C
ATOM   981  O   LEU A 147     32.914  40.466  31.364  1.00 70.81       O
ATOM   982  N   ILE A 148     30.914  39.855  32.198  1.00 70.62       N
ATOM   983  CA  ILE A 148     30.163  40.233  31.008  1.00 70.53       C
ATOM   984  CB  ILE A 148     28.669  39.878  31.172  1.00 70.38       C
ATOM   985  CG2 ILE A 148     27.858  40.466  30.025  1.00 70.25       C
ATOM   986  CG1 ILE A 148     28.506  38.358  31.229  1.00 70.30       C
ATOM   987  CD1 ILE A 148     27.075  37.894  31.422  1.00 70.22       C
ATOM   988  C   ILE A 148     30.285  41.723  30.701  1.00 70.59       C
ATOM   989  O   ILE A 148     30.228  42.135  29.543  1.00 70.52       O
ATOM   990  N   ALA A 149     30.457  42.527  31.743  1.00 70.67       N
ATOM   991  CA  ALA A 149     30.579  43.967  31.573  1.00 70.58       C
ATOM   992  CB  ALA A 149     29.961  44.681  32.769  1.00 70.60       C
ATOM   993  C   ALA A 149     32.034  44.392  31.402  1.00 70.54       C
ATOM   994  O   ALA A 149     32.323  45.395  30.747  1.00 70.64       O
ATOM   995  N   ARG A 150     32.948  43.620  31.979  1.00 70.38       N
ATOM   996  CA  ARG A 150     34.370  43.938  31.906  1.00 70.26       C
ATOM   997  CB  ARG A 150     35.140  43.138  32.964  1.00 70.67       C
ATOM   998  CG  ARG A 150     36.625  43.473  33.034  1.00 71.26       C
ATOM   999  CD  ARG A 150     37.341  42.765  34.186  1.00 71.83       C
ATOM  1000  NE  ARG A 150     36.910  43.228  35.505  1.00 72.23       N
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Figure 8S

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ATOM   1001  CZ  ARG A 150      35.813  42.811  36.134  1.00 72.55           C
ATOM   1002  NH1 ARG A 150      35.017  41.907  35.572  1.00 72.75           N
ATOM   1003  NH2 ARG A 150      35.511  43.299  37.331  1.00 72.57           N
ATOM   1004  C   ARG A 150      35.024  43.735  30.536  1.00 69.94           C
ATOM   1005  O   ARG A 150      35.754  44.611  30.063  1.00 69.86           O
ATOM   1006  N   PHE A 151      34.773  42.595  29.895  1.00 69.42           N
ATOM   1007  CA  PHE A 151      35.380  42.329  28.591  1.00 68.83           C
ATOM   1008  CB  PHE A 151      36.232  41.055  28.644  1.00 68.80           C
ATOM   1009  CG  PHE A 151      37.376  41.128  29.616  1.00 68.86           C
ATOM   1010  CD1 PHE A 151      37.245  40.621  30.905  1.00 68.95           C
ATOM   1011  CD2 PHE A 151      38.583  41.714  29.247  1.00 68.94           C
ATOM   1012  CE1 PHE A 151      38.302  40.696  31.813  1.00 68.85           C
ATOM   1013  CE2 PHE A 151      39.645  41.794  30.148  1.00 68.87           C
ATOM   1014  CZ  PHE A 151      39.503  41.284  31.432  1.00 68.86           C
ATOM   1015  C   PHE A 151      34.400  42.221  27.426  1.00 68.31           C
ATOM   1016  O   PHE A 151      34.789  41.836  26.324  1.00 68.27           O
ATOM   1017  N   ALA A 152      33.139  42.564  27.661  1.00 67.70           N
ATOM   1018  CA  ALA A 152      32.136  42.498  26.605  1.00 67.16           C
ATOM   1019  CB  ALA A 152      31.309  41.231  26.757  1.00 67.17           C
ATOM   1020  C   ALA A 152      31.229  43.725  26.621  1.00 66.73           C
ATOM   1021  O   ALA A 152      30.010  43.613  26.510  1.00 66.67           O
ATOM   1022  N   ASN A 153      31.838  44.899  26.751  1.00 66.39           N
ATOM   1023  CA  ASN A 153      31.098  46.156  26.791  1.00 65.89           C
ATOM   1024  CB  ASN A 153      31.966  47.243  27.436  1.00 66.36           C
ATOM   1025  CG  ASN A 153      31.191  48.517  27.732  1.00 66.81           C
ATOM   1026  OD1 ASN A 153      31.761  49.509  28.191  1.00 66.98           O
ATOM   1027  ND2 ASN A 153      29.886  48.495  27.478  1.00 66.94           N
ATOM   1028  C   ASN A 153      30.669  46.600  25.392  1.00 65.27           C
ATOM   1029  O   ASN A 153      29.718  47.364  25.237  1.00 65.39           O
ATOM   1030  N   GLU A 154      31.369  46.111  24.374  1.00 64.45           N
ATOM   1031  CA  GLU A 154      31.063  46.476  22.997  1.00 63.52           C
ATOM   1032  CB  GLU A 154      32.366  46.632  22.204  1.00 64.22           C
ATOM   1033  CG  GLU A 154      33.491  45.686  22.626  1.00 65.05           C
ATOM   1034  CD  GLU A 154      33.119  44.220  22.493  1.00 65.51           C
ATOM   1035  OE1 GLU A 154      32.757  43.794  21.373  1.00 65.78           O
ATOM   1036  OE2 GLU A 154      33.193  43.495  23.510  1.00 65.61           O
ATOM   1037  C   GLU A 154      30.121  45.519  22.269  1.00 62.47           C
ATOM   1038  O   GLU A 154      29.863  45.687  21.074  1.00 62.51           O
ATOM   1039  N   CYS A 155      29.602  44.522  22.981  1.00 60.87           N
ATOM   1040  CA  CYS A 155      28.684  43.561  22.373  1.00 59.19           C
ATOM   1041  CB  CYS A 155      29.437  42.294  21.950  1.00 59.45           C
ATOM   1042  SG  CYS A 155      30.164  41.355  23.315  1.00 59.76           S
ATOM   1043  C   CYS A 155      27.564  43.192  23.337  1.00 57.82           C
ATOM   1044  O   CYS A 155      27.679  43.403  24.541  1.00 57.62           O
ATOM   1045  N   GLN A 156      26.477  42.645  22.802  1.00 56.31           N
ATOM   1046  CA  GLN A 156      25.353  42.249  23.637  1.00 54.79           C
ATOM   1047  CB  GLN A 156      24.024  42.538  22.932  1.00 55.37           C
ATOM   1048  CG  GLN A 156      23.782  41.739  21.671  1.00 56.39           C
ATOM   1049  CD  GLN A 156      22.406  41.995  21.084  1.00 57.13           C
ATOM   1050  OE1 GLN A 156      22.079  43.123  20.703  1.00 57.59           O
ATOM   1051  NE2 GLN A 156      21.590  40.946  21.011  1.00 57.49           N
ATOM   1052  C   GLN A 156      25.457  40.767  23.976  1.00 53.29           C
ATOM   1053  O   GLN A 156      25.692  39.929  23.107  1.00 53.00           O
ATOM   1054  N   ILE A 157      25.275  40.453  25.252  1.00 51.67           N
ATOM   1055  CA  ILE A 157      25.372  39.081  25.720  1.00 49.85           C
ATOM   1056  CB  ILE A 157      26.185  39.009  27.030  1.00 50.01           C
ATOM   1057  CG2 ILE A 157      26.243  37.575  27.537  1.00 50.23           C
ATOM   1058  CG1 ILE A 157      27.589  39.570  26.801  1.00 50.25           C
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Figure 8T

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ATOM   1059  CD1 ILE A 157     28.382  38.852  25.727  1.00 50.65      C
ATOM   1060  C   ILE A 157     24.021  38.430  25.958  1.00 48.42      C
ATOM   1061  O   ILE A 157     23.185  38.955  26.689  1.00 48.14      O
ATOM   1062  N   GLU A 158     23.819  37.279  25.328  1.00 46.69      N
ATOM   1063  CA  GLU A 158     22.589  36.518  25.481  1.00 45.32      C
ATOM   1064  CB  GLU A 158     22.104  35.996  24.127  1.00 45.68      C
ATOM   1065  CG  GLU A 158     21.695  37.070  23.136  1.00 46.58      C
ATOM   1066  CD  GLU A 158     20.560  37.931  23.652  1.00 47.34      C
ATOM   1067  OE1 GLU A 158     19.576  37.369  24.179  1.00 47.28      O
ATOM   1068  OE2 GLU A 158     20.650  39.169  23.525  1.00 48.19      O
ATOM   1069  C   GLU A 158     22.920  35.336  26.385  1.00 43.98      C
ATOM   1070  O   GLU A 158     23.606  34.407  25.963  1.00 43.50      O
ATOM   1071  N   MET A 159     22.446  35.378  27.626  1.00 42.74      N
ATOM   1072  CA  MET A 159     22.711  34.295  28.570  1.00 41.56      C
ATOM   1073  CB  MET A 159     22.798  34.815  30.004  1.00 42.39      C
ATOM   1074  CG  MET A 159     24.088  35.514  30.371  1.00 44.11      C
ATOM   1075  SD  MET A 159     24.267  35.526  32.176  1.00 46.60      S
ATOM   1076  CE  MET A 159     22.851  36.541  32.649  1.00 46.03      C
ATOM   1077  C   MET A 159     21.648  33.218  28.532  1.00 40.26      C
ATOM   1078  O   MET A 159     20.464  33.501  28.365  1.00 39.98      O
ATOM   1079  N   LEU A 160     22.083  31.978  28.704  1.00 38.69      N
ATOM   1080  CA  LEU A 160     21.172  30.848  28.721  1.00 37.59      C
ATOM   1081  CB  LEU A 160     21.018  30.279  27.305  1.00 37.60      C
ATOM   1082  CG  LEU A 160     19.784  29.422  27.024  1.00 37.90      C
ATOM   1083  CD1 LEU A 160     19.650  29.202  25.519  1.00 37.83      C
ATOM   1084  CD2 LEU A 160     19.890  28.097  27.761  1.00 37.80      C
ATOM   1085  C   LEU A 160     21.750  29.800  29.677  1.00 36.65      C
ATOM   1086  O   LEU A 160     22.753  29.151  29.374  1.00 36.13      O
ATOM   1087  N   GLY A 161     21.125  29.663  30.844  1.00 35.74      N
ATOM   1088  CA  GLY A 161     21.586  28.699  31.831  1.00 34.53      C
ATOM   1089  C   GLY A 161     20.761  27.429  31.760  1.00 33.81      C
ATOM   1090  O   GLY A 161     19.531  27.483  31.773  1.00 33.71      O
ATOM   1091  N   SER A 162     21.424  26.281  31.688  1.00 32.70      N
ATOM   1092  CA  SER A 162     20.701  25.018  31.599  1.00 31.67      C
ATOM   1093  CB  SER A 162     20.570  24.587  30.134  1.00 30.98      C
ATOM   1094  OG  SER A 162     19.993  23.293  30.042  1.00 30.57      O
ATOM   1095  C   SER A 162     21.317  23.873  32.386  1.00 31.01      C
ATOM   1096  O   SER A 162     22.365  23.346  32.016  1.00 30.76      O
ATOM   1097  N   ALA A 163     20.650  23.477  33.464  1.00 30.33      N
ATOM   1098  CA  ALA A 163     21.125  22.369  34.273  1.00 29.58      C
ATOM   1099  CB  ALA A 163     20.385  22.341  35.603  1.00 30.07      C
ATOM   1100  C   ALA A 163     20.856  21.080  33.489  1.00 29.44      C
ATOM   1101  O   ALA A 163     21.569  20.089  33.631  1.00 28.92      O
ATOM   1102  N   GLU A 164     19.825  21.106  32.649  1.00 29.32      N
ATOM   1103  CA  GLU A 164     19.476  19.936  31.853  1.00 29.78      C
ATOM   1104  CB  GLU A 164     18.172  20.184  31.095  1.00 31.44      C
ATOM   1105  CG  GLU A 164     17.655  18.951  30.371  1.00 34.82      C
ATOM   1106  CD  GLU A 164     16.325  19.187  29.679  1.00 36.46      C
ATOM   1107  OE1 GLU A 164     15.678  20.222  29.958  1.00 38.07      O
ATOM   1108  OE2 GLU A 164     15.924  18.327  28.864  1.00 37.79      O
ATOM   1109  C   GLU A 164     20.582  19.575  30.859  1.00 29.30      C
ATOM   1110  O   GLU A 164     20.847  18.399  30.596  1.00 28.77      O
ATOM   1111  N   MET A 165     21.232  20.587  30.300  1.00 28.45      N
ATOM   1112  CA  MET A 165     22.298  20.317  29.345  1.00 28.20      C
ATOM   1113  CB  MET A 165     22.778  21.620  28.710  1.00 28.91      C
ATOM   1114  CG  MET A 165     23.570  21.398  27.431  1.00 30.59      C
ATOM   1115  SD  MET A 165     24.035  22.940  26.620  1.00 31.94      S
ATOM   1116  CE  MET A 165     22.494  23.418  25.882  1.00 31.97      C
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Figure 8U

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ATOM   1117  C   MET A 165     23.454  19.606  30.050  1.00 27.54      C
ATOM   1118  O   MET A 165     24.131  18.758  29.463  1.00 27.24      O
ATOM   1119  N   VAL A 166     23.678  19.952  31.314  1.00 26.73      N
ATOM   1120  CA  VAL A 166     24.740  19.311  32.073  1.00 26.74      C
ATOM   1121  CB  VAL A 166     24.841  19.883  33.500  1.00 26.61      C
ATOM   1122  CG1 VAL A 166     25.928  19.145  34.277  1.00 26.96      C
ATOM   1123  CG2 VAL A 166     25.149  21.373  33.441  1.00 26.49      C
ATOM   1124  C   VAL A 166     24.424  17.820  32.152  1.00 27.07      C
ATOM   1125  O   VAL A 166     25.301  16.980  31.972  1.00 26.02      O
ATOM   1126  N   GLU A 167     23.158  17.506  32.417  1.00 27.89      N
ATOM   1127  CA  GLU A 167     22.714  16.121  32.517  1.00 29.12      C
ATOM   1128  CB  GLU A 167     21.260  16.062  33.002  1.00 31.04      C
ATOM   1129  CG  GLU A 167     21.099  16.378  34.471  1.00 34.37      C
ATOM   1130  CD  GLU A 167     22.033  15.552  35.344  1.00 36.89      C
ATOM   1131  OE1 GLU A 167     22.130  14.321  35.130  1.00 38.46      O
ATOM   1132  OE2 GLU A 167     22.675  16.130  36.249  1.00 38.74      O
ATOM   1133  C   GLU A 167     22.842  15.390  31.189  1.00 28.28      C
ATOM   1134  O   GLU A 167     23.150  14.200  31.153  1.00 28.26      O
ATOM   1135  N   LEU A 168     22.598  16.100  30.095  1.00 28.21      N
ATOM   1136  CA  LEU A 168     22.712  15.494  28.779  1.00 28.05      C
ATOM   1137  CB  LEU A 168     22.265  16.487  27.697  1.00 28.07      C
ATOM   1138  CG  LEU A 168     20.756  16.747  27.683  1.00 28.26      C
ATOM   1139  CD1 LEU A 168     20.422  17.814  26.662  1.00 28.45      C
ATOM   1140  CD2 LEU A 168     20.025  15.452  27.366  1.00 28.49      C
ATOM   1141  C   LEU A 168     24.163  15.077  28.568  1.00 27.93      C
ATOM   1142  O   LEU A 168     24.438  13.999  28.037  1.00 28.11      O
ATOM   1143  N   ALA A 169     25.089  15.926  29.007  1.00 27.73      N
ATOM   1144  CA  ALA A 169     26.515  15.632  28.873  1.00 28.12      C
ATOM   1145  CB  ALA A 169     27.358  16.852  29.288  1.00 27.69      C
ATOM   1146  C   ALA A 169     26.859  14.426  29.746  1.00 28.18      C
ATOM   1147  O   ALA A 169     27.572  13.519  29.311  1.00 28.29      O
ATOM   1148  N   GLU A 170     26.357  14.415  30.978  1.00 28.76      N
ATOM   1149  CA  GLU A 170     26.610  13.285  31.873  1.00 29.18      C
ATOM   1150  CB  GLU A 170     25.898  13.480  33.218  1.00 29.14      C
ATOM   1151  CG  GLU A 170     26.581  14.460  34.167  1.00 29.02      C
ATOM   1152  CD  GLU A 170     27.862  13.903  34.788  1.00 29.97      C
ATOM   1153  OE1 GLU A 170     28.793  14.700  35.045  1.00 29.30      O
ATOM   1154  OE2 GLU A 170     27.939  12.676  35.032  1.00 30.01      O
ATOM   1155  C   GLU A 170     26.099  12.011  31.205  1.00 29.51      C
ATOM   1156  O   GLU A 170     26.824  11.025  31.090  1.00 29.71      O
ATOM   1157  N   ALA A 171     24.848  12.042  30.752  1.00 29.94      N
ATOM   1158  CA  ALA A 171     24.253  10.883  30.094  1.00 30.26      C
ATOM   1159  CB  ALA A 171     22.868  11.234  29.572  1.00 30.29      C
ATOM   1160  C   ALA A 171     25.124  10.394  28.947  1.00 30.81      C
ATOM   1161  O   ALA A 171     25.412   9.201  28.834  1.00 31.13      O
ATOM   1162  N   LYS A 172     25.546  11.316  28.091  1.00 31.06      N
ATOM   1163  CA  LYS A 172     26.366  10.947  26.950  1.00 32.12      C
ATOM   1164  CB  LYS A 172     26.795  12.192  26.171  1.00 32.06      C
ATOM   1165  CG  LYS A 172     27.626  11.871  24.940  1.00 32.46      C
ATOM   1166  CD  LYS A 172     28.013  13.136  24.180  1.00 32.50      C
ATOM   1167  CE  LYS A 172     28.815  12.800  22.932  1.00 33.01      C
ATOM   1168  NZ  LYS A 172     29.159  14.022  22.167  1.00 32.96      N
ATOM   1169  C   LYS A 172     27.597  10.131  27.326  1.00 32.64      C
ATOM   1170  O   LYS A 172     27.829   9.062  26.757  1.00 32.92      O
ATOM   1171  N   LEU A 173     28.387  10.620  28.276  1.00 33.14      N
ATOM   1172  CA  LEU A 173     29.587   9.897  28.669  1.00 34.31      C
ATOM   1173  CB  LEU A 173     30.552  10.812  29.433  1.00 34.17      C
ATOM   1174  CG  LEU A 173     31.093  12.078  28.747  1.00 34.37      C
```

Figure 8V

ATOM 1175 CD1 LEU A 173 32.576 12.212 29.062 1.00 33.96 C
ATOM 1176 CD2 LEU A 173 30.880 12.025 27.247 1.00 34.33 C
ATOM 1177 C LEU A 173 29.278 8.653 29.496 1.00 35.30 C
ATOM 1178 O LEU A 173 30.172 7.870 29.805 1.00 35.42 O
ATOM 1179 N HIS A 174 28.015 8.473 29.864 1.00 36.72 N
ATOM 1180 CA HIS A 174 27.630 7.293 30.626 1.00 38.16 C
ATOM 1181 CB HIS A 174 26.560 7.644 31.664 1.00 37.76 C
ATOM 1182 CG HIS A 174 27.124 8.213 32.929 1.00 37.39 C
ATOM 1183 CD2 HIS A 174 27.348 9.494 33.308 1.00 37.15 C
ATOM 1184 ND1 HIS A 174 27.602 7.422 33.953 1.00 37.82 N
ATOM 1185 CE1 HIS A 174 28.095 8.192 34.907 1.00 37.44 C
ATOM 1186 NE2 HIS A 174 27.955 9.453 34.540 1.00 37.12 N
ATOM 1187 C HIS A 174 27.130 6.219 29.669 1.00 39.31 C
ATOM 1188 O HIS A 174 26.810 5.108 30.083 1.00 39.72 O
ATOM 1189 N GLY A 175 27.073 6.560 28.384 1.00 40.42 N
ATOM 1190 CA GLY A 175 26.639 5.597 27.387 1.00 41.81 C
ATOM 1191 C GLY A 175 25.287 5.845 26.747 1.00 43.00 C
ATOM 1192 O GLY A 175 24.886 5.105 25.846 1.00 43.03 O
ATOM 1193 N GLU A 176 24.571 6.868 27.204 1.00 43.77 N
ATOM 1194 CA GLU A 176 23.266 7.173 26.629 1.00 45.02 C
ATOM 1195 CB GLU A 176 22.324 7.762 27.686 1.00 46.03 C
ATOM 1196 CG GLU A 176 21.921 6.795 28.792 1.00 47.96 C
ATOM 1197 CD GLU A 176 22.955 6.689 29.898 1.00 49.25 C
ATOM 1198 OE1 GLU A 176 23.169 7.694 30.614 1.00 49.83 O
ATOM 1199 OE2 GLU A 176 23.552 5.601 30.055 1.00 50.12 O
ATOM 1200 C GLU A 176 23.413 8.153 25.474 1.00 45.17 C
ATOM 1201 O GLU A 176 24.327 8.975 25.459 1.00 45.70 O
ATOM 1202 N ASP A 177 22.512 8.059 24.503 1.00 45.24 N
ATOM 1203 CA ASP A 177 22.545 8.938 23.342 1.00 44.89 C
ATOM 1204 CB ASP A 177 21.869 8.253 22.157 1.00 46.19 C
ATOM 1205 CG ASP A 177 22.460 6.882 21.871 1.00 47.31 C
ATOM 1206 OD1 ASP A 177 23.559 6.818 21.272 1.00 47.70 O
ATOM 1207 OD2 ASP A 177 21.831 5.873 22.257 1.00 48.01 O
ATOM 1208 C ASP A 177 21.833 10.238 23.672 1.00 43.98 C
ATOM 1209 O ASP A 177 20.814 10.243 24.357 1.00 44.07 O
ATOM 1210 N VAL A 178 22.381 11.342 23.186 1.00 42.87 N
ATOM 1211 CA VAL A 178 21.800 12.649 23.441 1.00 41.57 C
ATOM 1212 CB VAL A 178 22.852 13.765 23.229 1.00 41.43 C
ATOM 1213 CG1 VAL A 178 22.253 15.120 23.567 1.00 40.77 C
ATOM 1214 CG2 VAL A 178 24.035 13.484 24.083 1.00 41.33 C
ATOM 1215 C VAL A 178 20.608 12.913 22.524 1.00 40.74 C
ATOM 1216 O VAL A 178 20.715 12.801 21.305 1.00 40.65 O
ATOM 1217 N SER A 179 19.471 13.260 23.118 1.00 40.12 N
ATOM 1218 CA SER A 179 18.271 13.564 22.346 1.00 39.22 C
ATOM 1219 CB SER A 179 17.032 13.517 23.234 1.00 39.19 C
ATOM 1220 OG SER A 179 15.955 14.187 22.604 1.00 39.12 O
ATOM 1221 C SER A 179 18.397 14.957 21.751 1.00 38.78 C
ATOM 1222 O SER A 179 18.419 15.950 22.482 1.00 38.57 O
ATOM 1223 N LEU A 180 18.480 15.036 20.427 1.00 38.11 N
ATOM 1224 CA LEU A 180 18.602 16.330 19.772 1.00 37.12 C
ATOM 1225 CB LEU A 180 18.859 16.153 18.276 1.00 37.25 C
ATOM 1226 CG LEU A 180 20.159 15.430 17.903 1.00 37.36 C
ATOM 1227 CD1 LEU A 180 20.354 15.483 16.394 1.00 37.56 C
ATOM 1228 CD2 LEU A 180 21.344 16.082 18.615 1.00 37.57 C
ATOM 1229 C LEU A 180 17.355 17.173 19.995 1.00 36.72 C
ATOM 1230 O LEU A 180 17.433 18.398 20.045 1.00 36.33 O
ATOM 1231 N ASP A 181 16.203 16.523 20.136 1.00 36.44 N
ATOM 1232 CA ASP A 181 14.966 17.256 20.366 1.00 36.07 C

Figure 8W

ATOM 1233 CB ASP A 181 13.754 16.319 20.311 1.00 37.55 C
ATOM 1234 CG ASP A 181 13.486 15.790 18.909 1.00 38.95 C
ATOM 1235 OD1 ASP A 181 13.589 16.570 17.937 1.00 39.74 O
ATOM 1236 OD2 ASP A 181 13.158 14.594 18.777 1.00 40.38 O
ATOM 1237 C ASP A 181 15.014 17.971 21.714 1.00 34.99 C
ATOM 1238 O ASP A 181 14.491 19.074 21.859 1.00 34.62 O
ATOM 1239 N ALA A 182 15.638 17.337 22.702 1.00 34.20 N
ATOM 1240 CA ALA A 182 15.766 17.939 24.026 1.00 33.44 C
ATOM 1241 CB ALA A 182 16.388 16.937 25.003 1.00 33.26 C
ATOM 1242 C ALA A 182 16.645 19.186 23.910 1.00 32.88 C
ATOM 1243 O ALA A 182 16.362 20.216 24.514 1.00 32.37 O
ATOM 1244 N LEU A 183 17.714 19.085 23.124 1.00 32.52 N
ATOM 1245 CA LEU A 183 18.614 20.214 22.915 1.00 31.97 C
ATOM 1246 CB LEU A 183 19.823 19.796 22.080 1.00 32.53 C
ATOM 1247 CG LEU A 183 21.089 19.365 22.816 1.00 33.44 C
ATOM 1248 CD1 LEU A 183 22.184 19.088 21.785 1.00 33.67 C
ATOM 1249 CD2 LEU A 183 21.533 20.463 23.787 1.00 33.50 C
ATOM 1250 C LEU A 183 17.913 21.366 22.213 1.00 31.47 C
ATOM 1251 O LEU A 183 18.060 22.524 22.609 1.00 31.07 O
ATOM 1252 N LYS A 184 17.160 21.050 21.163 1.00 30.86 N
ATOM 1253 CA LYS A 184 16.443 22.075 20.413 1.00 31.16 C
ATOM 1254 CB LYS A 184 15.651 21.445 19.262 1.00 31.63 C
ATOM 1255 CG LYS A 184 16.513 20.868 18.158 1.00 32.93 C
ATOM 1256 CD LYS A 184 15.675 20.111 17.139 1.00 33.75 C
ATOM 1257 CE LYS A 184 16.556 19.416 16.115 1.00 34.92 C
ATOM 1258 NZ LYS A 184 15.750 18.568 15.178 1.00 35.78 N
ATOM 1259 C LYS A 184 15.487 22.824 21.328 1.00 30.89 C
ATOM 1260 O LYS A 184 15.307 24.033 21.199 1.00 30.37 O
ATOM 1261 N ARG A 185 14.869 22.090 22.244 1.00 30.97 N
ATOM 1262 CA ARG A 185 13.926 22.680 23.183 1.00 31.66 C
ATOM 1263 CB ARG A 185 13.260 21.576 24.011 1.00 32.95 C
ATOM 1264 CG ARG A 185 12.273 22.095 25.045 1.00 35.19 C
ATOM 1265 CD ARG A 185 11.071 22.763 24.385 1.00 36.95 C
ATOM 1266 NE ARG A 185 10.276 23.497 25.366 1.00 38.48 N
ATOM 1267 CZ ARG A 185 10.678 24.616 25.959 1.00 39.27 C
ATOM 1268 NH1 ARG A 185 11.864 25.138 25.668 1.00 39.25 N
ATOM 1269 NH2 ARG A 185 9.901 25.206 26.857 1.00 40.18 N
ATOM 1270 C ARG A 185 14.667 23.645 24.101 1.00 30.92 C
ATOM 1271 O ARG A 185 14.239 24.781 24.313 1.00 30.74 O
ATOM 1272 N ILE A 186 15.789 23.186 24.642 1.00 30.14 N
ATOM 1273 CA ILE A 186 16.585 24.022 25.528 1.00 29.32 C
ATOM 1274 CB ILE A 186 17.832 23.252 26.037 1.00 29.04 C
ATOM 1275 CG2 ILE A 186 18.741 24.190 26.829 1.00 29.20 C
ATOM 1276 CG1 ILE A 186 17.389 22.058 26.894 1.00 29.51 C
ATOM 1277 CD1 ILE A 186 18.534 21.148 27.330 1.00 29.37 C
ATOM 1278 C ILE A 186 17.037 25.285 24.792 1.00 28.71 C
ATOM 1279 O ILE A 186 17.015 26.380 25.351 1.00 28.31 O
ATOM 1280 N LEU A 187 17.435 25.130 23.532 1.00 28.36 N
ATOM 1281 CA LEU A 187 17.911 26.257 22.733 1.00 28.42 C
ATOM 1282 CB LEU A 187 18.998 25.772 21.757 1.00 28.23 C
ATOM 1283 CG LEU A 187 20.268 25.207 22.409 1.00 28.51 C
ATOM 1284 CD1 LEU A 187 21.125 24.483 21.376 1.00 28.72 C
ATOM 1285 CD2 LEU A 187 21.049 26.337 23.051 1.00 28.48 C
ATOM 1286 C LEU A 187 16.814 26.996 21.956 1.00 28.77 C
ATOM 1287 O LEU A 187 17.105 27.913 21.189 1.00 27.81 O
ATOM 1288 N ARG A 188 15.559 26.611 22.173 1.00 29.44 N
ATOM 1289 CA ARG A 188 14.437 27.232 21.470 1.00 30.59 C
ATOM 1290 CB ARG A 188 13.096 26.759 22.066 1.00 31.00 C

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Figure 8X

ATOM 1291 CG ARG A 188 11.880 27.044 21.161 1.00 31.92 C
ATOM 1292 CD ARG A 188 10.591 26.415 21.694 1.00 32.72 C
ATOM 1293 NE ARG A 188 10.065 27.111 22.869 1.00 33.40 N
ATOM 1294 CZ ARG A 188 8.896 26.834 23.440 1.00 33.80 C
ATOM 1295 NH1 ARG A 188 8.127 25.871 22.951 1.00 34.90 N
ATOM 1296 NH2 ARG A 188 8.486 27.525 24.492 1.00 34.07 N
ATOM 1297 C ARG A 188 14.522 28.761 21.479 1.00 31.15 C
ATOM 1298 O ARG A 188 14.384 29.394 20.437 1.00 31.37 O
ATOM 1299 N PRO A 189 14.778 29.373 22.652 1.00 31.69 N
ATOM 1300 CD PRO A 189 15.085 28.750 23.953 1.00 31.58 C
ATOM 1301 CA PRO A 189 14.877 30.835 22.741 1.00 32.00 C
ATOM 1302 CB PRO A 189 15.460 31.055 24.134 1.00 32.34 C
ATOM 1303 CG PRO A 189 14.931 29.907 24.908 1.00 32.12 C
ATOM 1304 C PRO A 189 15.781 31.423 21.661 1.00 32.69 C
ATOM 1305 O PRO A 189 15.444 32.428 21.024 1.00 33.41 O
ATOM 1306 N TRP A 190 16.937 30.795 21.467 1.00 32.33 N
ATOM 1307 CA TRP A 190 17.902 31.251 20.478 1.00 32.66 C
ATOM 1308 CB TRP A 190 19.276 30.637 20.767 1.00 31.96 C
ATOM 1309 CG TRP A 190 19.946 31.238 21.972 1.00 31.74 C
ATOM 1310 CD2 TRP A 190 21.261 30.942 22.461 1.00 31.19 C
ATOM 1311 CE2 TRP A 190 21.475 31.752 23.597 1.00 31.14 C
ATOM 1312 CE3 TRP A 190 22.278 30.070 22.048 1.00 31.17 C
ATOM 1313 CD1 TRP A 190 19.432 32.187 22.808 1.00 31.47 C
ATOM 1314 NE1 TRP A 190 20.343 32.502 23.786 1.00 31.75 N
ATOM 1315 CZ2 TRP A 190 22.666 31.719 24.327 1.00 30.64 C
ATOM 1316 CZ3 TRP A 190 23.468 30.038 22.777 1.00 30.63 C
ATOM 1317 CH2 TRP A 190 23.647 30.858 23.903 1.00 30.76 C
ATOM 1318 C TRP A 190 17.473 30.936 19.053 1.00 32.80 C
ATOM 1319 O TRP A 190 17.678 31.739 18.151 1.00 33.14 O
ATOM 1320 N LEU A 191 16.875 29.769 18.853 1.00 33.23 N
ATOM 1321 CA LEU A 191 16.420 29.384 17.525 1.00 34.12 C
ATOM 1322 CB LEU A 191 15.997 27.913 17.514 1.00 34.10 C
ATOM 1323 CG LEU A 191 17.133 26.920 17.767 1.00 34.63 C
ATOM 1324 CD1 LEU A 191 16.571 25.512 17.926 1.00 34.77 C
ATOM 1325 CD2 LEU A 191 18.124 26.985 16.605 1.00 34.84 C
ATOM 1326 C LEU A 191 15.264 30.262 17.047 1.00 34.32 C
ATOM 1327 O LEU A 191 14.943 30.270 15.864 1.00 34.60 O
ATOM 1328 N ARG A 192 14.640 31.000 17.962 1.00 34.66 N
ATOM 1329 CA ARG A 192 13.532 31.879 17.584 1.00 35.36 C
ATOM 1330 CB ARG A 192 12.417 31.827 18.630 1.00 35.21 C
ATOM 1331 CG ARG A 192 11.568 30.569 18.575 1.00 34.86 C
ATOM 1332 CD ARG A 192 10.556 30.560 19.709 1.00 34.91 C
ATOM 1333 NE ARG A 192 9.624 29.440 19.608 1.00 35.35 N
ATOM 1334 CZ ARG A 192 8.670 29.181 20.500 1.00 34.80 C
ATOM 1335 NH1 ARG A 192 8.528 29.960 21.563 1.00 34.29 N
ATOM 1336 NH2 ARG A 192 7.851 28.152 20.318 1.00 34.13 N
ATOM 1337 C ARG A 192 13.966 33.328 17.393 1.00 35.93 C
ATOM 1338 O ARG A 192 13.130 34.204 17.168 1.00 36.00 O
ATOM 1339 N MET A 193 15.270 33.579 17.479 1.00 36.28 N
ATOM 1340 CA MET A 193 15.797 34.930 17.316 1.00 36.54 C
ATOM 1341 CB MET A 193 17.139 35.070 18.045 1.00 36.79 C
ATOM 1342 CG MET A 193 17.038 35.165 19.564 1.00 36.88 C
ATOM 1343 SD MET A 193 18.669 35.278 20.352 1.00 37.53 S
ATOM 1344 CE MET A 193 19.079 37.031 20.122 1.00 36.86 C
ATOM 1345 C MET A 193 15.987 35.306 15.848 1.00 36.67 C
ATOM 1346 O MET A 193 16.368 34.467 15.025 1.00 36.46 O
ATOM 1347 N LYS A 194 15.715 36.570 15.526 1.00 37.01 N
ATOM 1348 CA LYS A 194 15.889 37.067 14.163 1.00 37.69 C

Figure 8Y

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ATOM  1349  CB  LYS A 194      15.478  38.545  14.064  1.00 38.05           C
ATOM  1350  CG  LYS A 194      15.613  39.121  12.654  1.00 38.80           C
ATOM  1351  CD  LYS A 194      16.261  40.515  12.623  1.00 39.92           C
ATOM  1352  CE  LYS A 194      15.284  41.663  12.887  1.00 40.54           C
ATOM  1353  NZ  LYS A 194      14.817  41.801  14.299  1.00 41.22           N
ATOM  1354  C   LYS A 194      17.374  36.928  13.832  1.00 37.73           C
ATOM  1355  O   LYS A 194      17.757  36.399  12.787  1.00 37.39           O
ATOM  1356  N   GLU A 195      18.206  37.413  14.744  1.00 38.33           N
ATOM  1357  CA  GLU A 195      19.650  37.332  14.574  1.00 38.43           C
ATOM  1358  CB  GLU A 195      20.248  38.722  14.361  1.00 39.41           C
ATOM  1359  CG  GLU A 195      21.766  38.698  14.281  1.00 41.23           C
ATOM  1360  CD  GLU A 195      22.348  39.961  13.690  1.00 42.54           C
ATOM  1361  OE1 GLU A 195      21.953  41.066  14.125  1.00 43.29           O
ATOM  1362  OE2 GLU A 195      23.211  39.844  12.792  1.00 43.45           O
ATOM  1363  C   GLU A 195      20.268  36.688  15.810  1.00 37.55           C
ATOM  1364  O   GLU A 195      20.596  37.368  16.781  1.00 37.40           O
ATOM  1365  N   PRO A 196      20.422  35.358  15.792  1.00 36.88           N
ATOM  1366  CD  PRO A 196      20.121  34.417  14.697  1.00 37.02           C
ATOM  1367  CA  PRO A 196      21.006  34.659  16.940  1.00 36.26           C
ATOM  1368  CB  PRO A 196      20.744  33.191  16.611  1.00 36.49           C
ATOM  1369  CG  PRO A 196      20.877  33.165  15.122  1.00 37.04           C
ATOM  1370  C   PRO A 196      22.491  34.973  17.078  1.00 35.39           C
ATOM  1371  O   PRO A 196      23.105  35.530  16.166  1.00 35.42           O
ATOM  1372  N   PRO A 197      23.089  34.626  18.228  1.00 34.89           N
ATOM  1373  CD  PRO A 197      22.518  33.900  19.374  1.00 34.65           C
ATOM  1374  CA  PRO A 197      24.517  34.894  18.438  1.00 34.16           C
ATOM  1375  CB  PRO A 197      24.789  34.288  19.820  1.00 34.06           C
ATOM  1376  CG  PRO A 197      23.457  34.284  20.480  1.00 34.48           C
ATOM  1377  C   PRO A 197      25.334  34.192  17.366  1.00 33.22           C
ATOM  1378  O   PRO A 197      25.018  33.067  16.991  1.00 33.54           O
ATOM  1379  N   ASP A 198      26.376  34.838  16.857  1.00 32.64           N
ATOM  1380  CA  ASP A 198      27.200  34.173  15.861  1.00 32.00           C
ATOM  1381  CB  ASP A 198      27.669  35.169  14.782  1.00 32.92           C
ATOM  1382  CG  ASP A 198      28.741  36.136  15.269  1.00 34.20           C
ATOM  1383  OD1 ASP A 198      28.889  36.334  16.497  1.00 34.32           O
ATOM  1384  OD2 ASP A 198      29.433  36.718  14.394  1.00 34.48           O
ATOM  1385  C   ASP A 198      28.379  33.517  16.590  1.00 30.70           C
ATOM  1386  O   ASP A 198      29.151  32.754  16.008  1.00 30.48           O
ATOM  1387  N   THR A 199      28.477  33.797  17.885  1.00 29.73           N
ATOM  1388  CA  THR A 199      29.541  33.245  18.728  1.00 28.32           C
ATOM  1389  CB  THR A 199      30.609  34.317  19.009  1.00 28.44           C
ATOM  1390  OG1 THR A 199      31.040  34.892  17.767  1.00 28.45           O
ATOM  1391  CG2 THR A 199      31.817  33.703  19.712  1.00 27.68           C
ATOM  1392  C   THR A 199      28.925  32.774  20.050  1.00 27.54           C
ATOM  1393  O   THR A 199      28.258  33.544  20.731  1.00 27.62           O
ATOM  1394  N   VAL A 200      29.137  31.509  20.408  1.00 26.67           N
ATOM  1395  CA  VAL A 200      28.573  30.975  21.645  1.00 25.45           C
ATOM  1396  CB  VAL A 200      27.603  29.794  21.368  1.00 25.29           C
ATOM  1397  CG1 VAL A 200      27.103  29.205  22.688  1.00 24.41           C
ATOM  1398  CG2 VAL A 200      26.410  30.273  20.533  1.00 25.16           C
ATOM  1399  C   VAL A 200      29.665  30.485  22.586  1.00 24.96           C
ATOM  1400  O   VAL A 200      30.457  29.615  22.228  1.00 25.00           O
ATOM  1401  N   VAL A 201      29.692  31.050  23.787  1.00 24.00           N
ATOM  1402  CA  VAL A 201      30.672  30.680  24.803  1.00 24.07           C
ATOM  1403  CB  VAL A 201      30.931  31.850  25.784  1.00 23.91           C
ATOM  1404  CG1 VAL A 201      31.872  31.401  26.907  1.00 23.25           C
ATOM  1405  CG2 VAL A 201      31.527  33.032  25.035  1.00 23.70           C
ATOM  1406  C   VAL A 201      30.151  29.506  25.620  1.00 23.96           C
```

Figure 8Z

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ATOM  1407  O   VAL A 201     29.044  29.551  26.144  1.00 24.03      O
ATOM  1408  N   LEU A 202     30.937  28.445  25.711  1.00 24.28      N
ATOM  1409  CA  LEU A 202     30.531  27.304  26.519  1.00 24.52      C
ATOM  1410  CB  LEU A 202     31.091  26.010  25.927  1.00 24.85      C
ATOM  1411  CG  LEU A 202     30.634  25.793  24.479  1.00 24.66      C
ATOM  1412  CD1 LEU A 202     31.126  24.450  23.954  1.00 25.52      C
ATOM  1413  CD2 LEU A 202     29.115  25.869  24.418  1.00 24.68      C
ATOM  1414  C   LEU A 202     31.123  27.596  27.890  1.00 24.97      C
ATOM  1415  O   LEU A 202     32.318  27.377  28.124  1.00 25.27      O
ATOM  1416  N   GLY A 203     30.283  28.132  28.772  1.00 25.47      N
ATOM  1417  CA  GLY A 203     30.708  28.498  30.114  1.00 26.68      C
ATOM  1418  C   GLY A 203     30.468  27.425  31.157  1.00 27.26      C
ATOM  1419  O   GLY A 203     30.282  27.711  32.337  1.00 28.58      O
ATOM  1420  N   CYS A 204     30.441  26.182  30.704  1.00 27.73      N
ATOM  1421  CA  CYS A 204     30.273  25.034  31.582  1.00 27.40      C
ATOM  1422  CB  CYS A 204     28.824  24.551  31.568  1.00 28.28      C
ATOM  1423  SG  CYS A 204     28.483  23.277  32.788  1.00 29.75      S
ATOM  1424  C   CYS A 204     31.200  23.998  30.959  1.00 26.65      C
ATOM  1425  O   CYS A 204     31.088  23.705  29.768  1.00 26.53      O
ATOM  1426  N   THR A 205     32.130  23.455  31.740  1.00 25.96      N
ATOM  1427  CA  THR A 205     33.072  22.481  31.188  1.00 25.54      C
ATOM  1428  CB  THR A 205     34.179  22.112  32.213  1.00 25.97      C
ATOM  1429  OG1 THR A 205     33.604  21.417  33.326  1.00 25.47      O
ATOM  1430  CG2 THR A 205     34.866  23.376  32.720  1.00 26.26      C
ATOM  1431  C   THR A 205     32.398  21.209  30.671  1.00 25.02      C
ATOM  1432  O   THR A 205     33.020  20.402  29.978  1.00 25.08      O
ATOM  1433  N   HIS A 206     31.126  21.024  31.004  1.00 25.00      N
ATOM  1434  CA  HIS A 206     30.389  19.861  30.507  1.00 25.50      C
ATOM  1435  CB  HIS A 206     29.096  19.644  31.301  1.00 25.48      C
ATOM  1436  CG  HIS A 206     29.243  18.752  32.496  1.00 25.77      C
ATOM  1437  CD2 HIS A 206     28.818  17.485  32.715  1.00 26.12      C
ATOM  1438  ND1 HIS A 206     29.853  19.158  33.664  1.00 26.12      N
ATOM  1439  CE1 HIS A 206     29.794  18.182  34.552  1.00 26.27      C
ATOM  1440  NE2 HIS A 206     29.171  17.156  34.001  1.00 25.97      N
ATOM  1441  C   HIS A 206     29.990  20.056  29.038  1.00 25.23      C
ATOM  1442  O   HIS A 206     29.915  19.096  28.261  1.00 24.85      O
ATOM  1443  N   PHE A 207     29.739  21.305  28.661  1.00 25.12      N
ATOM  1444  CA  PHE A 207     29.259  21.602  27.314  1.00 24.78      C
ATOM  1445  CB  PHE A 207     28.765  23.059  27.262  1.00 24.50      C
ATOM  1446  CG  PHE A 207     27.625  23.346  28.223  1.00 24.94      C
ATOM  1447  CD1 PHE A 207     27.171  24.651  28.422  1.00 24.92      C
ATOM  1448  CD2 PHE A 207     27.019  22.311  28.945  1.00 25.02      C
ATOM  1449  CE1 PHE A 207     26.137  24.924  29.322  1.00 24.91      C
ATOM  1450  CE2 PHE A 207     25.984  22.574  29.848  1.00 24.68      C
ATOM  1451  CZ  PHE A 207     25.544  23.881  30.037  1.00 24.50      C
ATOM  1452  C   PHE A 207     30.139  21.263  26.117  1.00 24.23      C
ATOM  1453  O   PHE A 207     29.624  20.794  25.105  1.00 24.49      O
ATOM  1454  N   PRO A 208     31.467  21.485  26.199  1.00 24.05      N
ATOM  1455  CD  PRO A 208     32.268  22.196  27.216  1.00 23.52      C
ATOM  1456  CA  PRO A 208     32.292  21.140  25.035  1.00 23.79      C
ATOM  1457  CB  PRO A 208     33.709  21.443  25.519  1.00 23.37      C
ATOM  1458  CG  PRO A 208     33.497  22.617  26.415  1.00 23.62      C
ATOM  1459  C   PRO A 208     32.111  19.665  24.650  1.00 23.75      C
ATOM  1460  O   PRO A 208     32.307  19.283  23.496  1.00 23.71      O
ATOM  1461  N   LEU A 209     31.731  18.846  25.628  1.00 24.35      N
ATOM  1462  CA  LEU A 209     31.510  17.416  25.400  1.00 24.73      C
ATOM  1463  CB  LEU A 209     31.225  16.703  26.730  1.00 24.44      C
ATOM  1464  CG  LEU A 209     32.351  16.705  27.763  1.00 24.17      C
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Figure 8AA

ATOM 1465 CD1 LEU A 209 31.856 16.084 29.055 1.00 24.39 C
ATOM 1466 CD2 LEU A 209 33.546 15.940 27.213 1.00 25.04 C
ATOM 1467 C LEU A 209 30.330 17.193 24.453 1.00 24.96 C
ATOM 1468 O LEU A 209 30.185 16.115 23.871 1.00 25.40 O
ATOM 1469 N LEU A 210 29.492 18.214 24.311 1.00 25.40 N
ATOM 1470 CA LEU A 210 28.313 18.150 23.445 1.00 26.09 C
ATOM 1471 CB LEU A 210 27.091 18.700 24.187 1.00 26.08 C
ATOM 1472 CG LEU A 210 26.612 17.931 25.424 1.00 26.43 C
ATOM 1473 CD1 LEU A 210 25.590 18.754 26.165 1.00 26.49 C
ATOM 1474 CD2 LEU A 210 26.031 16.587 25.006 1.00 26.75 C
ATOM 1475 C LEU A 210 28.513 18.956 22.165 1.00 26.97 C
ATOM 1476 O LEU A 210 27.551 19.238 21.443 1.00 26.49 O
ATOM 1477 N GLN A 211 29.754 19.325 21.877 1.00 27.84 N
ATOM 1478 CA GLN A 211 30.018 20.125 20.689 1.00 29.76 C
ATOM 1479 CB GLN A 211 31.525 20.241 20.426 1.00 31.43 C
ATOM 1480 CG GLN A 211 31.822 21.058 19.169 1.00 35.04 C
ATOM 1481 CD GLN A 211 33.278 21.444 19.027 1.00 36.79 C
ATOM 1482 OE1 GLN A 211 33.814 22.205 19.840 1.00 38.21 O
ATOM 1483 NE2 GLN A 211 33.929 20.926 17.985 1.00 37.92 N
ATOM 1484 C GLN A 211 29.319 19.624 19.428 1.00 29.78 C
ATOM 1485 O GLN A 211 28.629 20.390 18.757 1.00 29.75 O
ATOM 1486 N GLU A 212 29.482 18.346 19.104 1.00 30.23 N
ATOM 1487 CA GLU A 212 28.857 17.805 17.898 1.00 31.41 C
ATOM 1488 CB GLU A 212 29.173 16.312 17.750 1.00 33.48 C
ATOM 1489 CG GLU A 212 28.789 15.739 16.391 1.00 36.83 C
ATOM 1490 CD GLU A 212 29.709 14.609 15.940 1.00 38.98 C
ATOM 1491 OE1 GLU A 212 30.921 14.860 15.738 1.00 40.36 O
ATOM 1492 OE2 GLU A 212 29.223 13.468 15.786 1.00 40.67 O
ATOM 1493 C GLU A 212 27.348 18.023 17.894 1.00 30.99 C
ATOM 1494 O GLU A 212 26.791 18.548 16.928 1.00 30.68 O
ATOM 1495 N GLU A 213 26.692 17.628 18.983 1.00 30.23 N
ATOM 1496 CA GLU A 213 25.253 17.788 19.103 1.00 29.95 C
ATOM 1497 CB GLU A 213 24.760 17.214 20.436 1.00 30.26 C
ATOM 1498 CG GLU A 213 24.844 15.697 20.570 1.00 31.58 C
ATOM 1499 CD GLU A 213 26.237 15.179 20.909 1.00 32.64 C
ATOM 1500 OE1 GLU A 213 27.150 15.992 21.177 1.00 32.85 O
ATOM 1501 OE2 GLU A 213 26.412 13.942 20.915 1.00 33.12 O
ATOM 1502 C GLU A 213 24.840 19.258 19.005 1.00 29.41 C
ATOM 1503 O GLU A 213 23.857 19.587 18.338 1.00 29.01 O
ATOM 1504 N LEU A 214 25.580 20.137 19.681 1.00 28.84 N
ATOM 1505 CA LEU A 214 25.268 21.567 19.656 1.00 28.43 C
ATOM 1506 CB LEU A 214 26.216 22.348 20.570 1.00 28.13 C
ATOM 1507 CG LEU A 214 25.977 22.173 22.075 1.00 27.63 C
ATOM 1508 CD1 LEU A 214 27.109 22.818 22.862 1.00 27.49 C
ATOM 1509 CD2 LEU A 214 24.626 22.791 22.447 1.00 27.85 C
ATOM 1510 C LEU A 214 25.348 22.136 18.247 1.00 28.83 C
ATOM 1511 O LEU A 214 24.507 22.937 17.845 1.00 27.87 O
ATOM 1512 N LEU A 215 26.356 21.713 17.498 1.00 29.30 N
ATOM 1513 CA LEU A 215 26.528 22.202 16.142 1.00 30.96 C
ATOM 1514 CB LEU A 215 27.918 21.822 15.630 1.00 30.54 C
ATOM 1515 CG LEU A 215 29.025 22.593 16.358 1.00 30.81 C
ATOM 1516 CD1 LEU A 215 30.386 22.124 15.895 1.00 30.80 C
ATOM 1517 CD2 LEU A 215 28.858 24.084 16.093 1.00 30.46 C
ATOM 1518 C LEU A 215 25.440 21.709 15.191 1.00 31.93 C
ATOM 1519 O LEU A 215 25.211 22.308 14.145 1.00 32.43 O
ATOM 1520 N GLN A 216 24.762 20.625 15.551 1.00 33.13 N
ATOM 1521 CA GLN A 216 23.695 20.108 14.701 1.00 34.56 C
ATOM 1522 CB GLN A 216 23.435 18.625 14.988 1.00 35.66 C

Figure 8BB

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ATOM  1523  CG  GLN A 216      24.610  17.700  14.728  1.00 37.89           C
ATOM  1524  CD  GLN A 216      24.241  16.238  14.906  1.00 39.33           C
ATOM  1525  OE1 GLN A 216      23.524  15.665  14.083  1.00 41.09           O
ATOM  1526  NE2 GLN A 216      24.717  15.629  15.988  1.00 39.66           N
ATOM  1527  C   GLN A 216      22.406  20.888  14.939  1.00 34.80           C
ATOM  1528  O   GLN A 216      21.569  21.014  14.047  1.00 35.06           O
ATOM  1529  N   VAL A 217      22.258  21.416  16.148  1.00 34.71           N
ATOM  1530  CA  VAL A 217      21.064  22.156  16.531  1.00 35.07           C
ATOM  1531  CB  VAL A 217      20.710  21.866  18.016  1.00 35.06           C
ATOM  1532  CG1 VAL A 217      19.504  22.685  18.451  1.00 35.49           C
ATOM  1533  CG2 VAL A 217      20.435  20.390  18.192  1.00 35.11           C
ATOM  1534  C   VAL A 217      21.164  23.664  16.336  1.00 35.24           C
ATOM  1535  O   VAL A 217      20.199  24.304  15.925  1.00 34.92           O
ATOM  1536  N   LEU A 218      22.326  24.233  16.640  1.00 35.48           N
ATOM  1537  CA  LEU A 218      22.520  25.674  16.511  1.00 35.98           C
ATOM  1538  CB  LEU A 218      23.837  26.097  17.175  1.00 35.20           C
ATOM  1539  CG  LEU A 218      23.954  25.958  18.699  1.00 34.74           C
ATOM  1540  CD1 LEU A 218      25.415  26.086  19.099  1.00 33.85           C
ATOM  1541  CD2 LEU A 218      23.107  27.018  19.395  1.00 34.29           C
ATOM  1542  C   LEU A 218      22.520  26.143  15.059  1.00 36.85           C
ATOM  1543  O   LEU A 218      22.923  25.408  14.154  1.00 36.56           O
ATOM  1544  N   PRO A 219      22.062  27.382  14.819  1.00 37.78           N
ATOM  1545  CD  PRO A 219      21.542  28.360  15.788  1.00 38.25           C
ATOM  1546  CA  PRO A 219      22.026  27.929  13.461  1.00 38.69           C
ATOM  1547  CB  PRO A 219      21.507  29.354  13.664  1.00 38.57           C
ATOM  1548  CG  PRO A 219      21.840  29.660  15.088  1.00 38.75           C
ATOM  1549  C   PRO A 219      23.390  27.895  12.785  1.00 39.23           C
ATOM  1550  O   PRO A 219      24.422  28.136  13.419  1.00 39.41           O
ATOM  1551  N   GLU A 220      23.381  27.591  11.494  1.00 39.72           N
ATOM  1552  CA  GLU A 220      24.600  27.502  10.698  1.00 40.27           C
ATOM  1553  CB  GLU A 220      24.250  27.481   9.207  1.00 41.80           C
ATOM  1554  CG  GLU A 220      22.941  26.777   8.874  1.00 43.87           C
ATOM  1555  CD  GLU A 220      22.413  27.165   7.498  1.00 45.18           C
ATOM  1556  OE1 GLU A 220      23.087  26.854   6.492  1.00 45.89           O
ATOM  1557  OE2 GLU A 220      21.325  27.789   7.425  1.00 45.96           O
ATOM  1558  C   GLU A 220      25.505  28.698  10.972  1.00 39.71           C
ATOM  1559  O   GLU A 220      25.023  29.808  11.211  1.00 40.05           O
ATOM  1560  N   GLY A 221      26.813  28.466  10.946  1.00 38.99           N
ATOM  1561  CA  GLY A 221      27.758  29.547  11.162  1.00 38.23           C
ATOM  1562  C   GLY A 221      28.059  29.947  12.595  1.00 37.79           C
ATOM  1563  O   GLY A 221      28.875  30.842  12.818  1.00 37.76           O
ATOM  1564  N   THR A 222      27.414  29.308  13.566  1.00 36.92           N
ATOM  1565  CA  THR A 222      27.669  29.637  14.967  1.00 36.06           C
ATOM  1566  CB  THR A 222      26.600  29.039  15.911  1.00 36.28           C
ATOM  1567  OG1 THR A 222      25.286  29.441  15.489  1.00 35.84           O
ATOM  1568  CG2 THR A 222      26.836  29.530  17.331  1.00 35.92           C
ATOM  1569  C   THR A 222      29.031  29.082  15.375  1.00 35.26           C
ATOM  1570  O   THR A 222      29.325  27.904  15.159  1.00 35.42           O
ATOM  1571  N   ARG A 223      29.864  29.934  15.962  1.00 33.89           N
ATOM  1572  CA  ARG A 223      31.187  29.515  16.395  1.00 32.73           C
ATOM  1573  CB  ARG A 223      32.213  30.593  16.048  1.00 33.48           C
ATOM  1574  CG  ARG A 223      33.634  30.257  16.448  1.00 34.74           C
ATOM  1575  CD  ARG A 223      34.572  31.304  15.885  1.00 35.80           C
ATOM  1576  NE  ARG A 223      35.976  31.038  16.180  1.00 36.83           N
ATOM  1577  CZ  ARG A 223      36.975  31.735  15.653  1.00 36.90           C
ATOM  1578  NH1 ARG A 223      36.709  32.722  14.808  1.00 37.42           N
ATOM  1579  NH2 ARG A 223      38.229  31.460  15.974  1.00 37.62           N
ATOM  1580  C   ARG A 223      31.204  29.254  17.896  1.00 31.22           C
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Figure 8CC

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ATOM  1581  O   ARG A 223     30.823  30.118  18.684  1.00 31.14           O
ATOM  1582  N   LEU A 224     31.649  28.063  18.287  1.00 29.77           N
ATOM  1583  CA  LEU A 224     31.714  27.702  19.698  1.00 28.63           C
ATOM  1584  CB  LEU A 224     31.501  26.196  19.885  1.00 28.14           C
ATOM  1585  CG  LEU A 224     30.191  25.617  19.343  1.00 28.31           C
ATOM  1586  CD1 LEU A 224     30.145  24.122  19.618  1.00 27.77           C
ATOM  1587  CD2 LEU A 224     29.011  26.321  19.990  1.00 28.16           C
ATOM  1588  C   LEU A 224     33.074  28.088  20.267  1.00 28.22           C
ATOM  1589  O   LEU A 224     34.113  27.855  19.646  1.00 27.72           O
ATOM  1590  N   VAL A 225     33.055  28.678  21.452  1.00 27.59           N
ATOM  1591  CA  VAL A 225     34.279  29.094  22.114  1.00 27.22           C
ATOM  1592  CB  VAL A 225     34.386  30.638  22.165  1.00 27.19           C
ATOM  1593  CG1 VAL A 225     35.669  31.047  22.875  1.00 27.27           C
ATOM  1594  CG2 VAL A 225     34.346  31.219  20.755  1.00 27.27           C
ATOM  1595  C   VAL A 225     34.315  28.573  23.553  1.00 27.00           C
ATOM  1596  O   VAL A 225     33.343  28.707  24.291  1.00 26.02           O
ATOM  1597  N   ASP A 226     35.427  27.965  23.946  1.00 27.26           N
ATOM  1598  CA  ASP A 226     35.555  27.505  25.319  1.00 28.37           C
ATOM  1599  CB  ASP A 226     35.210  26.008  25.469  1.00 29.27           C
ATOM  1600  CG  ASP A 226     36.130  25.095  24.689  1.00 30.58           C
ATOM  1601  OD1 ASP A 226     37.361  25.166  24.874  1.00 31.43           O
ATOM  1602  OD2 ASP A 226     35.613  24.283  23.891  1.00 32.27           O
ATOM  1603  C   ASP A 226     36.952  27.818  25.835  1.00 28.68           C
ATOM  1604  O   ASP A 226     37.767  28.418  25.126  1.00 28.29           O
ATOM  1605  N   SER A 227     37.222  27.409  27.067  1.00 29.15           N
ATOM  1606  CA  SER A 227     38.493  27.693  27.730  1.00 30.16           C
ATOM  1607  CB  SER A 227     38.212  28.003  29.200  1.00 30.84           C
ATOM  1608  OG  SER A 227     37.330  29.105  29.315  1.00 33.08           O
ATOM  1609  C   SER A 227     39.568  26.613  27.662  1.00 29.90           C
ATOM  1610  O   SER A 227     40.696  26.833  28.118  1.00 30.24           O
ATOM  1611  N   GLY A 228     39.221  25.467  27.089  1.00 29.54           N
ATOM  1612  CA  GLY A 228     40.133  24.333  27.004  1.00 29.07           C
ATOM  1613  C   GLY A 228     41.586  24.537  26.605  1.00 29.10           C
ATOM  1614  O   GLY A 228     42.494  24.267  27.400  1.00 28.05           O
ATOM  1615  N   ALA A 229     41.810  24.983  25.368  1.00 28.66           N
ATOM  1616  CA  ALA A 229     43.161  25.208  24.868  1.00 28.46           C
ATOM  1617  CB  ALA A 229     43.113  25.634  23.399  1.00 28.89           C
ATOM  1618  C   ALA A 229     43.900  26.257  25.694  1.00 28.23           C
ATOM  1619  O   ALA A 229     45.095  26.127  25.934  1.00 28.75           O
ATOM  1620  N   ALA A 230     43.191  27.290  26.135  1.00 28.21           N
ATOM  1621  CA  ALA A 230     43.820  28.341  26.937  1.00 28.47           C
ATOM  1622  CB  ALA A 230     42.872  29.512  27.106  1.00 28.62           C
ATOM  1623  C   ALA A 230     44.248  27.821  28.309  1.00 29.04           C
ATOM  1624  O   ALA A 230     45.253  28.281  28.871  1.00 28.26           O
ATOM  1625  N   ILE A 231     43.476  26.874  28.850  1.00 28.95           N
ATOM  1626  CA  ILE A 231     43.785  26.281  30.149  1.00 29.12           C
ATOM  1627  CB  ILE A 231     42.651  25.351  30.636  1.00 29.08           C
ATOM  1628  CG2 ILE A 231     43.053  24.671  31.953  1.00 28.24           C
ATOM  1629  CG1 ILE A 231     41.364  26.152  30.804  1.00 29.21           C
ATOM  1630  CD1 ILE A 231     41.467  27.238  31.820  1.00 28.47           C
ATOM  1631  C   ILE A 231     45.035  25.442  29.986  1.00 29.33           C
ATOM  1632  O   ILE A 231     45.915  25.428  30.850  1.00 29.46           O
ATOM  1633  N   ALA A 232     45.097  24.729  28.870  1.00 29.68           N
ATOM  1634  CA  ALA A 232     46.237  23.884  28.566  1.00 30.26           C
ATOM  1635  CB  ALA A 232     46.030  23.206  27.223  1.00 30.00           C
ATOM  1636  C   ALA A 232     47.493  24.764  28.538  1.00 31.19           C
ATOM  1637  O   ALA A 232     48.487  24.458  29.202  1.00 31.16           O
ATOM  1638  N   ARG A 233     47.437  25.863  27.784  1.00 31.62           N
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Figure 8DD

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ATOM  1639  CA  ARG A 233      48.576  26.776  27.695  1.00 32.55           C
ATOM  1640  CB  ARG A 233      48.273  27.932  26.729  1.00 32.86           C
ATOM  1641  CG  ARG A 233      48.187  27.516  25.259  1.00 32.98           C
ATOM  1642  CD  ARG A 233      48.181  28.745  24.352  1.00 34.06           C
ATOM  1643  NE  ARG A 233      46.982  29.563  24.530  1.00 34.89           N
ATOM  1644  CZ  ARG A 233      45.818  29.316  23.934  1.00 35.40           C
ATOM  1645  NH1 ARG A 233      45.697  28.281  23.115  1.00 35.59           N
ATOM  1646  NH2 ARG A 233      44.770  30.094  24.168  1.00 35.89           N
ATOM  1647  C   ARG A 233      48.952  27.332  29.069  1.00 32.57           C
ATOM  1648  O   ARG A 233      50.129  27.422  29.402  1.00 32.69           O
ATOM  1649  N   ARG A 234      47.957  27.702  29.869  1.00 32.61           N
ATOM  1650  CA  ARG A 234      48.229  28.229  31.206  1.00 32.84           C
ATOM  1651  CB  ARG A 234      46.934  28.713  31.861  1.00 32.78           C
ATOM  1652  CG  ARG A 234      47.107  29.235  33.280  1.00 33.27           C
ATOM  1653  CD  ARG A 234      48.098  30.400  33.357  1.00 33.63           C
ATOM  1654  NE  ARG A 234      48.091  31.010  34.685  1.00 34.67           N
ATOM  1655  CZ  ARG A 234      48.883  32.009  35.060  1.00 34.84           C
ATOM  1656  NH1 ARG A 234      49.759  32.519  34.204  1.00 35.01           N
ATOM  1657  NH2 ARG A 234      48.794  32.502  36.289  1.00 35.15           N
ATOM  1658  C   ARG A 234      48.885  27.155  32.082  1.00 33.23           C
ATOM  1659  O   ARG A 234      49.760  27.458  32.901  1.00 33.10           O
ATOM  1660  N   THR A 235      48.464  25.906  31.897  1.00 32.93           N
ATOM  1661  CA  THR A 235      49.007  24.778  32.652  1.00 33.19           C
ATOM  1662  CB  THR A 235      48.201  23.486  32.368  1.00 32.74           C
ATOM  1663  OG1 THR A 235      46.879  23.637  32.899  1.00 32.01           O
ATOM  1664  CG2 THR A 235      48.867  22.262  33.013  1.00 32.30           C
ATOM  1665  C   THR A 235      50.475  24.564  32.290  1.00 33.74           C
ATOM  1666  O   THR A 235      51.327  24.396  33.170  1.00 33.08           O
ATOM  1667  N   ALA A 236      50.767  24.586  30.993  1.00 34.60           N
ATOM  1668  CA  ALA A 236      52.135  24.415  30.519  1.00 35.65           C
ATOM  1669  CB  ALA A 236      52.163  24.387  28.994  1.00 35.86           C
ATOM  1670  C   ALA A 236      53.021  25.548  31.042  1.00 36.35           C
ATOM  1671  O   ALA A 236      54.180  25.328  31.388  1.00 36.64           O
ATOM  1672  N   TRP A 237      52.480  26.761  31.109  1.00 37.16           N
ATOM  1673  CA  TRP A 237      53.261  27.893  31.599  1.00 38.00           C
ATOM  1674  CB  TRP A 237      52.509  29.208  31.380  1.00 38.98           C
ATOM  1675  CG  TRP A 237      53.355  30.429  31.649  1.00 40.50           C
ATOM  1676  CD2 TRP A 237      53.400  31.199  32.859  1.00 40.98           C
ATOM  1677  CE2 TRP A 237      54.352  32.228  32.667  1.00 41.43           C
ATOM  1678  CE3 TRP A 237      52.730  31.120  34.087  1.00 41.27           C
ATOM  1679  CD1 TRP A 237      54.260  31.006  30.797  1.00 41.31           C
ATOM  1680  NE1 TRP A 237      54.861  32.088  31.402  1.00 41.47           N
ATOM  1681  CZ2 TRP A 237      54.650  33.171  33.659  1.00 41.56           C
ATOM  1682  CZ3 TRP A 237      53.028  32.058  35.075  1.00 41.51           C
ATOM  1683  CH2 TRP A 237      53.980  33.070  34.852  1.00 41.65           C
ATOM  1684  C   TRP A 237      53.573  27.744  33.092  1.00 38.01           C
ATOM  1685  O   TRP A 237      54.687  28.035  33.537  1.00 37.78           O
ATOM  1686  N   LEU A 238      52.585  27.299  33.862  1.00 37.56           N
ATOM  1687  CA  LEU A 238      52.762  27.127  35.299  1.00 37.57           C
ATOM  1688  CB  LEU A 238      51.408  26.902  35.975  1.00 36.67           C
ATOM  1689  CG  LEU A 238      50.478  28.114  35.957  1.00 36.43           C
ATOM  1690  CD1 LEU A 238      49.116  27.731  36.487  1.00 36.24           C
ATOM  1691  CD2 LEU A 238      51.077  29.235  36.794  1.00 36.56           C
ATOM  1692  C   LEU A 238      53.703  25.977  35.622  1.00 37.81           C
ATOM  1693  O   LEU A 238      54.461  26.040  36.591  1.00 37.91           O
ATOM  1694  N   LEU A 239      53.660  24.923  34.819  1.00 38.48           N
ATOM  1695  CA  LEU A 239      54.540  23.791  35.057  1.00 39.58           C
ATOM  1696  CB  LEU A 239      54.163  22.619  34.149  1.00 39.09           C
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Figure 8EE

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ATOM  1697  CG  LEU A 239      52.839  21.921  34.493  1.00 38.87           C
ATOM  1698  CD1 LEU A 239      52.520  20.870  33.447  1.00 38.45           C
ATOM  1699  CD2 LEU A 239      52.936  21.293  35.881  1.00 38.47           C
ATOM  1700  C   LEU A 239      55.979  24.224  34.791  1.00 40.79           C
ATOM  1701  O   LEU A 239      56.927  23.586  35.249  1.00 40.92           O
ATOM  1702  N   GLU A 240      56.129  25.324  34.060  1.00 41.65           N
ATOM  1703  CA  GLU A 240      57.448  25.837  33.719  1.00 42.84           C
ATOM  1704  CB  GLU A 240      57.444  26.409  32.297  1.00 43.65           C
ATOM  1705  CG  GLU A 240      57.275  25.369  31.200  1.00 45.38           C
ATOM  1706  CD  GLU A 240      58.319  24.268  31.280  1.00 46.58           C
ATOM  1707  OE1 GLU A 240      59.529  24.596  31.325  1.00 47.04           O
ATOM  1708  OE2 GLU A 240      57.929  23.076  31.296  1.00 47.22           O
ATOM  1709  C   GLU A 240      57.961  26.905  34.667  1.00 43.09           C
ATOM  1710  O   GLU A 240      59.150  26.944  34.968  1.00 43.08           O
ATOM  1711  N   HIS A 241      57.069  27.767  35.143  1.00 43.49           N
ATOM  1712  CA  HIS A 241      57.486  28.858  36.011  1.00 44.38           C
ATOM  1713  CB  HIS A 241      57.070  30.186  35.364  1.00 45.65           C
ATOM  1714  CG  HIS A 241      57.586  30.367  33.967  1.00 47.27           C
ATOM  1715  CD2 HIS A 241      58.415  29.604  33.215  1.00 47.86           C
ATOM  1716  ND1 HIS A 241      57.237  31.442  33.178  1.00 47.83           N
ATOM  1717  CE1 HIS A 241      57.825  31.332  32.000  1.00 48.31           C
ATOM  1718  NE2 HIS A 241      58.546  30.225  31.996  1.00 48.70           N
ATOM  1719  C   HIS A 241      57.024  28.846  37.473  1.00 44.07           C
ATOM  1720  O   HIS A 241      57.400  29.741  38.232  1.00 44.13           O
ATOM  1721  N   GLU A 242      56.236  27.853  37.886  1.00 43.53           N
ATOM  1722  CA  GLU A 242      55.754  27.839  39.269  1.00 42.98           C
ATOM  1723  CB  GLU A 242      54.421  28.589  39.359  1.00 43.70           C
ATOM  1724  CG  GLU A 242      54.522  30.087  39.173  1.00 44.78           C
ATOM  1725  CD  GLU A 242      53.167  30.759  39.210  1.00 45.69           C
ATOM  1726  OE1 GLU A 242      52.341  30.397  40.081  1.00 45.73           O
ATOM  1727  OE2 GLU A 242      52.930  31.658  38.375  1.00 46.45           O
ATOM  1728  C   GLU A 242      55.578  26.498  39.977  1.00 42.31           C
ATOM  1729  O   GLU A 242      55.680  26.430  41.200  1.00 42.11           O
ATOM  1730  N   ALA A 243      55.306  25.439  39.224  1.00 41.35           N
ATOM  1731  CA  ALA A 243      55.072  24.127  39.820  1.00 40.63           C
ATOM  1732  CB  ALA A 243      54.557  23.163  38.758  1.00 40.62           C
ATOM  1733  C   ALA A 243      56.262  23.498  40.540  1.00 40.38           C
ATOM  1734  O   ALA A 243      57.382  23.480  40.025  1.00 39.78           O
ATOM  1735  N   PRO A 244      56.028  22.970  41.753  1.00 39.91           N
ATOM  1736  CD  PRO A 244      54.781  23.031  42.540  1.00 39.77           C
ATOM  1737  CA  PRO A 244      57.102  22.331  42.518  1.00 39.80           C
ATOM  1738  CB  PRO A 244      56.495  22.194  43.914  1.00 39.91           C
ATOM  1739  CG  PRO A 244      55.026  21.998  43.617  1.00 39.75           C
ATOM  1740  C   PRO A 244      57.415  20.982  41.875  1.00 39.90           C
ATOM  1741  O   PRO A 244      56.603  20.452  41.114  1.00 39.34           O
ATOM  1742  N   ASP A 245      58.588  20.431  42.176  1.00 40.00           N
ATOM  1743  CA  ASP A 245      59.011  19.149  41.615  1.00 40.24           C
ATOM  1744  CB  ASP A 245      60.516  18.947  41.853  1.00 41.09           C
ATOM  1745  CG  ASP A 245      61.071  17.750  41.102  1.00 41.84           C
ATOM  1746  OD1 ASP A 245      62.133  17.226  41.501  1.00 42.48           O
ATOM  1747  OD2 ASP A 245      60.455  17.334  40.100  1.00 42.69           O
ATOM  1748  C   ASP A 245      58.245  17.957  42.193  1.00 40.06           C
ATOM  1749  O   ASP A 245      58.817  17.131  42.907  1.00 40.25           O
ATOM  1750  N   ALA A 246      56.954  17.864  41.882  1.00 39.77           N
ATOM  1751  CA  ALA A 246      56.121  16.765  42.364  1.00 39.54           C
ATOM  1752  CB  ALA A 246      54.836  17.313  42.982  1.00 39.39           C
ATOM  1753  C   ALA A 246      55.796  15.857  41.182  1.00 39.56           C
ATOM  1754  O   ALA A 246      54.964  16.194  40.338  1.00 39.19           O
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Figure 8FF

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ATOM  1755 N   LYS A 247     56.446  14.699  41.129  1.00 39.47           N
ATOM  1756 CA  LYS A 247     56.245  13.771  40.024  1.00 39.58           C
ATOM  1757 CB  LYS A 247     57.416  13.892  39.049  1.00 40.22           C
ATOM  1758 CG  LYS A 247     58.777  13.707  39.705  1.00 41.70           C
ATOM  1759 CD  LYS A 247     59.910  13.916  38.706  1.00 43.00           C
ATOM  1760 CE  LYS A 247     61.266  13.866  39.394  1.00 43.78           C
ATOM  1761 NZ  LYS A 247     61.482  12.561  40.080  1.00 45.10           N
ATOM  1762 C   LYS A 247     56.097  12.317  40.450  1.00 39.34           C
ATOM  1763 O   LYS A 247     56.453  11.941  41.564  1.00 39.51           O
ATOM  1764 N   SER A 248     55.583  11.499  39.539  1.00 38.98           N
ATOM  1765 CA  SER A 248     55.385  10.082  39.793  1.00 38.69           C
ATOM  1766 CB  SER A 248     54.009   9.856  40.435  1.00 38.62           C
ATOM  1767 OG  SER A 248     53.728   8.479  40.587  1.00 38.23           O
ATOM  1768 C   SER A 248     55.487   9.286  38.492  1.00 38.63           C
ATOM  1769 O   SER A 248     55.262   9.820  37.405  1.00 38.34           O
ATOM  1770 N   ALA A 249     55.830   8.007  38.609  1.00 38.50           N
ATOM  1771 CA  ALA A 249     55.941   7.150  37.438  1.00 38.58           C
ATOM  1772 CB  ALA A 249     57.195   6.275  37.536  1.00 38.58           C
ATOM  1773 C   ALA A 249     54.691   6.281  37.308  1.00 38.38           C
ATOM  1774 O   ALA A 249     54.529   5.558  36.326  1.00 38.36           O
ATOM  1775 N   ASP A 250     53.805   6.357  38.299  1.00 38.17           N
ATOM  1776 CA  ASP A 250     52.572   5.576  38.269  1.00 37.75           C
ATOM  1777 CB  ASP A 250     51.765   5.767  39.562  1.00 38.49           C
ATOM  1778 CG  ASP A 250     52.435   5.136  40.773  1.00 39.62           C
ATOM  1779 OD1 ASP A 250     53.432   4.403  40.593  1.00 40.12           O
ATOM  1780 OD2 ASP A 250     51.960   5.365  41.909  1.00 39.88           O
ATOM  1781 C   ASP A 250     51.722   5.995  37.076  1.00 36.87           C
ATOM  1782 O   ASP A 250     51.859   7.106  36.563  1.00 37.25           O
ATOM  1783 N   ALA A 251     50.845   5.100  36.636  1.00 36.01           N
ATOM  1784 CA  ALA A 251     49.971   5.379  35.504  1.00 34.97           C
ATOM  1785 CB  ALA A 251     49.359   4.086  34.990  1.00 35.52           C
ATOM  1786 C   ALA A 251     48.868   6.349  35.918  1.00 33.97           C
ATOM  1787 O   ALA A 251     48.624   6.547  37.107  1.00 33.63           O
ATOM  1788 N   ASN A 252     48.206   6.948  34.933  1.00 32.74           N
ATOM  1789 CA  ASN A 252     47.131   7.894  35.204  1.00 31.53           C
ATOM  1790 CB  ASN A 252     46.550   8.451  33.903  1.00 31.29           C
ATOM  1791 CG  ASN A 252     47.583   9.156  33.059  1.00 31.11           C
ATOM  1792 OD1 ASN A 252     48.532   9.745  33.580  1.00 30.92           O
ATOM  1793 ND2 ASN A 252     47.397   9.118  31.747  1.00 31.17           N
ATOM  1794 C   ASN A 252     46.025   7.202  35.983  1.00 30.57           C
ATOM  1795 O   ASN A 252     45.737   6.032  35.755  1.00 30.37           O
ATOM  1796 N   ILE A 253     45.398   7.929  36.896  1.00 29.76           N
ATOM  1797 CA  ILE A 253     44.331   7.340  37.694  1.00 29.03           C
ATOM  1798 CB  ILE A 253     44.880   6.919  39.080  1.00 29.45           C
ATOM  1799 CG2 ILE A 253     45.374   8.139  39.833  1.00 29.70           C
ATOM  1800 CG1 ILE A 253     43.802   6.198  39.888  1.00 30.29           C
ATOM  1801 CD1 ILE A 253     44.292   5.736  41.244  1.00 31.33           C
ATOM  1802 C   ILE A 253     43.141   8.286  37.875  1.00 28.11           C
ATOM  1803 O   ILE A 253     43.297   9.512  37.893  1.00 27.59           O
ATOM  1804 N   ALA A 254     41.948   7.705  37.979  1.00 26.97           N
ATOM  1805 CA  ALA A 254     40.733   8.479  38.183  1.00 25.96           C
ATOM  1806 CB  ALA A 254     39.685   8.123  37.125  1.00 25.54           C
ATOM  1807 C   ALA A 254     40.200   8.167  39.578  1.00 25.64           C
ATOM  1808 O   ALA A 254     40.217   7.010  40.013  1.00 25.40           O
ATOM  1809 N   PHE A 255     39.749   9.203  40.276  1.00 24.93           N
ATOM  1810 CA  PHE A 255     39.188   9.061  41.619  1.00 25.25           C
ATOM  1811 CB  PHE A 255     39.931   9.936  42.633  1.00 24.82           C
ATOM  1812 CG  PHE A 255     41.278   9.416  43.044  1.00 25.59           C
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Figure 8GG

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ATOM  1813 CD1 PHE A 255     42.399  10.235  42.953  1.00 25.46       C
ATOM  1814 CD2 PHE A 255     41.422   8.132  43.559  1.00 26.01       C
ATOM  1815 CE1 PHE A 255     43.650   9.789  43.368  1.00 26.29       C
ATOM  1816 CE2 PHE A 255     42.671   7.668  43.982  1.00 26.91       C
ATOM  1817 CZ  PHE A 255     43.790   8.500  43.884  1.00 26.72       C
ATOM  1818 C   PHE A 255     37.726   9.503  41.663  1.00 25.33       C
ATOM  1819 O   PHE A 255     37.370  10.562  41.140  1.00 25.42       O
ATOM  1820 N   CYS A 256     36.874   8.698  42.284  1.00 25.82       N
ATOM  1821 CA  CYS A 256     35.482   9.099  42.462  1.00 26.46       C
ATOM  1822 CB  CYS A 256     34.512   8.041  41.920  1.00 27.23       C
ATOM  1823 SG  CYS A 256     34.653   6.407  42.664  1.00 29.02       S
ATOM  1824 C   CYS A 256     35.364   9.237  43.983  1.00 26.79       C
ATOM  1825 O   CYS A 256     36.246   8.775  44.715  1.00 26.33       O
ATOM  1826 N   MET A 257     34.308   9.877  44.475  1.00 27.23       N
ATOM  1827 CA  MET A 257     34.174  10.030  45.924  1.00 27.99       C
ATOM  1828 CB  MET A 257     33.566  11.395  46.270  1.00 28.01       C
ATOM  1829 CG  MET A 257     34.365  12.586  45.730  1.00 28.41       C
ATOM  1830 SD  MET A 257     36.165  12.503  46.030  1.00 29.78       S
ATOM  1831 CE  MET A 257     36.802  12.840  44.372  1.00 29.70       C
ATOM  1832 C   MET A 257     33.343   8.903  46.536  1.00 28.39       C
ATOM  1833 O   MET A 257     33.310   8.733  47.754  1.00 28.39       O
ATOM  1834 N   ALA A 258     32.691   8.128  45.679  1.00 29.08       N
ATOM  1835 CA  ALA A 258     31.880   6.999  46.117  1.00 30.02       C
ATOM  1836 CB  ALA A 258     30.474   7.460  46.494  1.00 29.75       C
ATOM  1837 C   ALA A 258     31.814   6.007  44.969  1.00 30.76       C
ATOM  1838 O   ALA A 258     31.509   6.379  43.837  1.00 30.44       O
ATOM  1839 N   MET A 259     32.111   4.747  45.259  1.00 31.73       N
ATOM  1840 CA  MET A 259     32.084   3.712  44.236  1.00 32.90       C
ATOM  1841 CB  MET A 259     32.945   2.527  44.675  1.00 34.30       C
ATOM  1842 CG  MET A 259     33.303   1.566  43.559  1.00 36.54       C
ATOM  1843 SD  MET A 259     34.242   2.358  42.237  1.00 38.48       S
ATOM  1844 CE  MET A 259     35.844   2.502  42.974  1.00 37.84       C
ATOM  1845 C   MET A 259     30.638   3.283  44.029  1.00 33.14       C
ATOM  1846 O   MET A 259     30.189   2.272  44.569  1.00 33.45       O
ATOM  1847 N   THR A 260     29.912   4.076  43.250  1.00 32.81       N
ATOM  1848 CA  THR A 260     28.509   3.827  42.955  1.00 32.55       C
ATOM  1849 CB  THR A 260     27.706   5.132  42.987  1.00 32.69       C
ATOM  1850 OG1 THR A 260     28.140   5.973  41.907  1.00 32.32       O
ATOM  1851 CG2 THR A 260     27.911   5.857  44.304  1.00 32.38       C
ATOM  1852 C   THR A 260     28.362   3.260  41.551  1.00 32.45       C
ATOM  1853 O   THR A 260     29.311   3.264  40.765  1.00 32.43       O
ATOM  1854 N   PRO A 261     27.165   2.765  41.212  1.00 32.43       N
ATOM  1855 CD  PRO A 261     26.012   2.408  42.064  1.00 32.73       C
ATOM  1856 CA  PRO A 261     27.002   2.227  39.862  1.00 32.04       C
ATOM  1857 CB  PRO A 261     25.559   1.726  39.864  1.00 32.40       C
ATOM  1858 CG  PRO A 261     25.383   1.268  41.293  1.00 32.56       C
ATOM  1859 C   PRO A 261     27.244   3.333  38.835  1.00 31.88       C
ATOM  1860 O   PRO A 261     27.850   3.096  37.796  1.00 31.83       O
ATOM  1861 N   GLY A 262     26.779   4.545  39.139  1.00 31.39       N
ATOM  1862 CA  GLY A 262     26.971   5.660  38.225  1.00 30.93       C
ATOM  1863 C   GLY A 262     28.439   5.941  37.935  1.00 30.03       C
ATOM  1864 O   GLY A 262     28.831   6.103  36.782  1.00 30.46       O
ATOM  1865 N   ALA A 263     29.254   6.003  38.980  1.00 29.43       N
ATOM  1866 CA  ALA A 263     30.678   6.248  38.816  1.00 28.87       C
ATOM  1867 CB  ALA A 263     31.342   6.409  40.178  1.00 28.90       C
ATOM  1868 C   ALA A 263     31.329   5.099  38.052  1.00 28.88       C
ATOM  1869 O   ALA A 263     32.162   5.314  37.170  1.00 28.36       O
ATOM  1870 N   GLU A 264     30.944   3.874  38.396  1.00 28.76       N
```

Figure 8HH

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ATOM  1871  CA  GLU A 264      31.505   2.691  37.752  1.00 29.21      C
ATOM  1872  CB  GLU A 264      30.980   1.432  38.457  1.00 29.05      C
ATOM  1873  CG  GLU A 264      31.358   1.396  39.931  1.00 29.36      C
ATOM  1874  CD  GLU A 264      30.506   0.450  40.767  1.00 29.84      C
ATOM  1875  OE1 GLU A 264      29.389   0.097  40.345  1.00 29.77      O
ATOM  1876  OE2 GLU A 264      30.955   0.080  41.870  1.00 30.70      O
ATOM  1877  C   GLU A 264      31.187   2.662  36.258  1.00 29.35      C
ATOM  1878  O   GLU A 264      32.006   2.220  35.451  1.00 29.37      O
ATOM  1879  N   GLN A 265      30.010   3.157  35.892  1.00 29.70      N
ATOM  1880  CA  GLN A 265      29.601   3.179  34.495  1.00 30.44      C
ATOM  1881  CB  GLN A 265      28.137   3.606  34.381  1.00 31.82      C
ATOM  1882  CG  GLN A 265      27.210   2.667  35.117  1.00 35.27      C
ATOM  1883  CD  GLN A 265      25.751   3.021  34.954  1.00 37.03      C
ATOM  1884  OE1 GLN A 265      24.889   2.428  35.607  1.00 39.00      O
ATOM  1885  NE2 GLN A 265      25.459   3.984  34.078  1.00 38.41      N
ATOM  1886  C   GLN A 265      30.474   4.076  33.621  1.00 29.94      C
ATOM  1887  O   GLN A 265      30.392   4.015  32.396  1.00 29.87      O
ATOM  1888  N   LEU A 266      31.299   4.906  34.247  1.00 29.15      N
ATOM  1889  CA  LEU A 266      32.198   5.791  33.506  1.00 29.01      C
ATOM  1890  CB  LEU A 266      32.496   7.055  34.318  1.00 28.73      C
ATOM  1891  CG  LEU A 266      31.367   8.075  34.425  1.00 29.05      C
ATOM  1892  CD1 LEU A 266      31.842   9.274  35.237  1.00 28.78      C
ATOM  1893  CD2 LEU A 266      30.937   8.502  33.024  1.00 28.78      C
ATOM  1894  C   LEU A 266      33.523   5.113  33.169  1.00 28.86      C
ATOM  1895  O   LEU A 266      34.319   5.643  32.386  1.00 28.44      O
ATOM  1896  N   LEU A 267      33.757   3.939  33.751  1.00 28.56      N
ATOM  1897  CA  LEU A 267      35.010   3.232  33.533  1.00 28.80      C
ATOM  1898  CB  LEU A 267      34.943   1.824  34.133  1.00 29.49      C
ATOM  1899  CG  LEU A 267      36.275   1.073  34.136  1.00 29.76      C
ATOM  1900  CD1 LEU A 267      37.305   1.829  34.979  1.00 29.91      C
ATOM  1901  CD2 LEU A 267      36.058  -0.329  34.700  1.00 30.42      C
ATOM  1902  C   LEU A 267      35.483   3.150  32.080  1.00 28.65      C
ATOM  1903  O   LEU A 267      36.609   3.529  31.782  1.00 28.27      O
ATOM  1904  N   PRO A 268      34.635   2.655  31.161  1.00 28.76      N
ATOM  1905  CD  PRO A 268      33.250   2.185  31.327  1.00 29.21      C
ATOM  1906  CA  PRO A 268      35.058   2.559  29.759  1.00 29.10      C
ATOM  1907  CB  PRO A 268      33.849   1.920  29.074  1.00 29.23      C
ATOM  1908  CG  PRO A 268      32.695   2.343  29.937  1.00 29.74      C
ATOM  1909  C   PRO A 268      35.470   3.902  29.135  1.00 29.03      C
ATOM  1910  O   PRO A 268      36.458   3.971  28.408  1.00 28.44      O
ATOM  1911  N   VAL A 269      34.719   4.961  29.422  1.00 29.23      N
ATOM  1912  CA  VAL A 269      35.045   6.283  28.885  1.00 29.50      C
ATOM  1913  CB  VAL A 269      33.888   7.279  29.118  1.00 30.12      C
ATOM  1914  CG1 VAL A 269      34.278   8.681  28.649  1.00 31.29      C
ATOM  1915  CG2 VAL A 269      32.667   6.812  28.338  1.00 31.48      C
ATOM  1916  C   VAL A 269      36.328   6.791  29.536  1.00 29.16      C
ATOM  1917  O   VAL A 269      37.220   7.299  28.852  1.00 29.31      O
ATOM  1918  N   LEU A 270      36.438   6.635  30.853  1.00 28.36      N
ATOM  1919  CA  LEU A 270      37.640   7.062  31.547  1.00 28.07      C
ATOM  1920  CB  LEU A 270      37.531   6.749  33.048  1.00 27.79      C
ATOM  1921  CG  LEU A 270      36.555   7.621  33.858  1.00 27.73      C
ATOM  1922  CD1 LEU A 270      36.423   7.075  35.273  1.00 26.65      C
ATOM  1923  CD2 LEU A 270      37.060   9.062  33.893  1.00 27.37      C
ATOM  1924  C   LEU A 270      38.859   6.358  30.942  1.00 28.42      C
ATOM  1925  O   LEU A 270      39.918   6.968  30.759  1.00 28.07      O
ATOM  1926  N   GLN A 271      38.706   5.075  30.620  1.00 28.62      N
ATOM  1927  CA  GLN A 271      39.803   4.309  30.036  1.00 29.58      C
ATOM  1928  CB  GLN A 271      39.446   2.815  30.009  1.00 29.77      C
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Figure 8II

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ATOM  1929 CG  GLN A 271    39.562  2.171 31.395  1.00 29.56      C
ATOM  1930 CD  GLN A 271    39.100  0.719 31.441  1.00 30.15      C
ATOM  1931 OE1 GLN A 271    39.476 -0.030 32.346  1.00 30.14      O
ATOM  1932 NE2 GLN A 271    38.276  0.322 30.480  1.00 29.92      N
ATOM  1933 C   GLN A 271    40.154  4.831 28.641  1.00 30.09      C
ATOM  1934 O   GLN A 271    41.333  4.935 28.298  1.00 30.05      O
ATOM  1935 N   ARG A 272    39.139  5.173 27.850  1.00 30.62      N
ATOM  1936 CA  ARG A 272    39.372  5.733 26.519  1.00 32.09      C
ATOM  1937 CB  ARG A 272    38.051  5.959 25.769  1.00 33.56      C
ATOM  1938 CG  ARG A 272    37.497  4.712 25.080  1.00 36.87      C
ATOM  1939 CD  ARG A 272    36.510  5.071 23.966  1.00 39.07      C
ATOM  1940 NE  ARG A 272    35.236  5.575 24.474  1.00 41.31      N
ATOM  1941 CZ  ARG A 272    34.331  4.826 25.101  1.00 42.35      C
ATOM  1942 NH1 ARG A 272    34.557  3.529 25.295  1.00 42.99      N
ATOM  1943 NH2 ARG A 272    33.201  5.372 25.538  1.00 42.53      N
ATOM  1944 C   ARG A 272    40.119  7.066 26.646  1.00 31.71      C
ATOM  1945 O   ARG A 272    40.888  7.441 25.758  1.00 31.85      O
ATOM  1946 N   TYR A 273    39.892  7.775 27.751  1.00 31.12      N
ATOM  1947 CA  TYR A 273    40.560  9.053 27.996  1.00 30.49      C
ATOM  1948 CB  TYR A 273    39.764  9.912 28.988  1.00 30.13      C
ATOM  1949 CG  TYR A 273    38.764 10.843 28.338  1.00 30.08      C
ATOM  1950 CD1 TYR A 273    37.423 10.485 28.209  1.00 30.27      C
ATOM  1951 CE1 TYR A 273    36.506 11.337 27.600  1.00 30.56      C
ATOM  1952 CD2 TYR A 273    39.165 12.084 27.840  1.00 30.11      C
ATOM  1953 CE2 TYR A 273    38.257 12.944 27.231  1.00 30.62      C
ATOM  1954 CZ  TYR A 273    36.932 12.566 27.113  1.00 31.12      C
ATOM  1955 OH  TYR A 273    36.035 13.413 26.506  1.00 31.48      O
ATOM  1956 C   TYR A 273    41.992  8.902 28.510  1.00 30.66      C
ATOM  1957 O   TYR A 273    42.738  9.878 28.577  1.00 30.68      O
ATOM  1958 N   GLY A 274    42.383  7.687 28.879  1.00 30.61      N
ATOM  1959 CA  GLY A 274    43.740  7.489 29.356  1.00 30.77      C
ATOM  1960 C   GLY A 274    43.881  7.150 30.830  1.00 31.11      C
ATOM  1961 O   GLY A 274    44.991  7.138 31.358  1.00 30.91      O
ATOM  1962 N   PHE A 275    42.766  6.888 31.503  1.00 31.47      N
ATOM  1963 CA  PHE A 275    42.810  6.527 32.918  1.00 32.19      C
ATOM  1964 CB  PHE A 275    41.801  7.348 33.728  1.00 31.21      C
ATOM  1965 CG  PHE A 275    42.032  8.831 33.653  1.00 30.69      C
ATOM  1966 CD1 PHE A 275    41.342  9.611 32.729  1.00 30.41      C
ATOM  1967 CD2 PHE A 275    42.970  9.441 34.477  1.00 29.75      C
ATOM  1968 CE1 PHE A 275    41.587 10.983 32.624  1.00 30.10      C
ATOM  1969 CE2 PHE A 275    43.223 10.809 34.382  1.00 30.33      C
ATOM  1970 CZ  PHE A 275    42.529 11.582 33.451  1.00 30.15      C
ATOM  1971 C   PHE A 275    42.471  5.048 33.007  1.00 33.19      C
ATOM  1972 O   PHE A 275    41.321  4.655 32.821  1.00 33.75      O
ATOM  1973 N   GLU A 276    43.484  4.234 33.277  1.00 34.59      N
ATOM  1974 CA  GLU A 276    43.310  2.789 33.361  1.00 36.07      C
ATOM  1975 CB  GLU A 276    44.675  2.103 33.438  1.00 37.83      C
ATOM  1976 CG  GLU A 276    45.583  2.659 34.528  1.00 39.84      C
ATOM  1977 CD  GLU A 276    46.443  1.587 35.173  1.00 41.24      C
ATOM  1978 OE1 GLU A 276    46.984  0.727 34.439  1.00 42.52      O
ATOM  1979 OE2 GLU A 276    46.588  1.607 36.415  1.00 41.91      O
ATOM  1980 C   GLU A 276    42.478  2.336 34.544  1.00 35.79      C
ATOM  1981 O   GLU A 276    41.703  1.381 34.442  1.00 35.99      O
ATOM  1982 N   THR A 277    42.632  3.035 35.662  1.00 35.29      N
ATOM  1983 CA  THR A 277    41.938  2.665 36.885  1.00 35.33      C
ATOM  1984 CB  THR A 277    42.976  2.238 37.953  1.00 35.95      C
ATOM  1985 OG1 THR A 277    43.827  1.222 37.404  1.00 37.35      O
ATOM  1986 CG2 THR A 277    42.292  1.707 39.198  1.00 36.44      C
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Figure 8JJ

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ATOM  1987  C   THR A 277     41.056   3.753  37.487  1.00 34.38      C
ATOM  1988  O   THR A 277     41.325   4.946  37.339  1.00 33.90      O
ATOM  1989  N   LEU A 278     39.999   3.309  38.162  1.00 33.42      N
ATOM  1990  CA  LEU A 278     39.063   4.180  38.860  1.00 32.84      C
ATOM  1991  CB  LEU A 278     37.660   4.078  38.261  1.00 32.25      C
ATOM  1992  CG  LEU A 278     36.557   4.754  39.080  1.00 31.65      C
ATOM  1993  CD1 LEU A 278     36.739   6.269  39.067  1.00 31.85      C
ATOM  1994  CD2 LEU A 278     35.204   4.385  38.506  1.00 32.00      C
ATOM  1995  C   LEU A 278     39.029   3.683  40.301  1.00 32.90      C
ATOM  1996  O   LEU A 278     38.696   2.523  40.551  1.00 32.50      O
ATOM  1997  N   GLU A 279     39.390   4.549  41.242  1.00 32.79      N
ATOM  1998  CA  GLU A 279     39.390   4.191  42.657  1.00 33.18      C
ATOM  1999  CB  GLU A 279     40.821   4.141  43.212  1.00 33.85      C
ATOM  2000  CG  GLU A 279     41.704   3.034  42.652  1.00 34.93      C
ATOM  2001  CD  GLU A 279     43.103   3.054  43.243  1.00 35.80      C
ATOM  2002  OE1 GLU A 279     43.990   2.345  42.711  1.00 37.17      O
ATOM  2003  OE2 GLU A 279     43.323   3.773  44.242  1.00 35.89      O
ATOM  2004  C   GLU A 279     38.596   5.205  43.472  1.00 33.21      C
ATOM  2005  O   GLU A 279     38.373   6.340  43.037  1.00 31.95      O
ATOM  2006  N   LYS A 280     38.173   4.786  44.660  1.00 33.51      N
ATOM  2007  CA  LYS A 280     37.438   5.666  45.550  1.00 34.17      C
ATOM  2008  CB  LYS A 280     36.529   4.868  46.489  1.00 34.76      C
ATOM  2009  CG  LYS A 280     35.955   5.721  47.620  1.00 35.25      C
ATOM  2010  CD  LYS A 280     34.963   4.950  48.463  1.00 36.16      C
ATOM  2011  CE  LYS A 280     34.444   5.796  49.618  1.00 36.76      C
ATOM  2012  NZ  LYS A 280     33.323   5.103  50.330  1.00 37.23      N
ATOM  2013  C   LYS A 280     38.437   6.456  46.382  1.00 34.45      C
ATOM  2014  O   LYS A 280     39.405   5.901  46.896  1.00 34.38      O
ATOM  2015  N   LEU A 281     38.204   7.756  46.503  1.00 34.75      N
ATOM  2016  CA  LEU A 281     39.079   8.605  47.293  1.00 35.65      C
ATOM  2017  CB  LEU A 281     39.370   9.908  46.550  1.00 35.08      C
ATOM  2018  CG  LEU A 281     40.280  10.898  47.278  1.00 34.82      C
ATOM  2019  CD1 LEU A 281     41.691  10.337  47.360  1.00 34.07      C
ATOM  2020  CD2 LEU A 281     40.273  12.230  46.537  1.00 34.40      C
ATOM  2021  C   LEU A 281     38.392   8.920  48.618  1.00 36.70      C
ATOM  2022  O   LEU A 281     37.230   9.325  48.635  1.00 36.57      O
ATOM  2023  N   ALA A 282     39.105   8.726  49.722  1.00 37.88      N
ATOM  2024  CA  ALA A 282     38.551   9.008  51.045  1.00 39.41      C
ATOM  2025  CB  ALA A 282     39.297   8.204  52.111  1.00 39.19      C
ATOM  2026  C   ALA A 282     38.687  10.501  51.327  1.00 40.14      C
ATOM  2027  O   ALA A 282     39.798  11.023  51.394  1.00 40.34      O
ATOM  2028  N   VAL A 283     37.556  11.179  51.500  1.00 41.23      N
ATOM  2029  CA  VAL A 283     37.550  12.617  51.757  1.00 42.40      C
ATOM  2030  CB  VAL A 283     36.640  13.340  50.746  1.00 42.15      C
ATOM  2031  CG1 VAL A 283     36.654  14.834  51.008  1.00 42.12      C
ATOM  2032  CG2 VAL A 283     37.097  13.037  49.330  1.00 42.22      C
ATOM  2033  C   VAL A 283     37.073  12.974  53.168  1.00 43.56      C
ATOM  2034  O   VAL A 283     36.188  12.315  53.718  1.00 43.82      O
ATOM  2035  N   LEU A 284     37.658  14.025  53.743  1.00 44.69      N
ATOM  2036  CA  LEU A 284     37.290  14.488  55.084  1.00 45.88      C
ATOM  2037  CB  LEU A 284     38.534  14.635  55.968  1.00 46.17      C
ATOM  2038  CG  LEU A 284     39.537  13.487  56.073  1.00 46.66      C
ATOM  2039  CD1 LEU A 284     40.567  13.830  57.143  1.00 46.97      C
ATOM  2040  CD2 LEU A 284     38.822  12.191  56.420  1.00 46.95      C
ATOM  2041  C   LEU A 284     36.591  15.844  55.006  1.00 46.59      C
ATOM  2042  O   LEU A 284     36.980  16.790  55.699  1.00 47.10      O
ATOM  2043  N   GLY A 285     35.567  15.945  54.165  1.00 47.04      N
ATOM  2044  CA  GLY A 285     34.858  17.204  54.025  1.00 47.76      C
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Figure 8KK

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ATOM  2045  C   GLY A 285     33.866  17.240  52.875  1.00 47.90      C
ATOM  2046  O   GLY A 285     32.783  17.840  53.035  1.00 48.58      O
ATOM  2047  OXT GLY A 285     34.176  16.690  51.803  1.00 48.12      O
ATOM  2048  N1  GLL H   1     31.450  21.033  34.964  1.00 27.57      N
ATOM  2049  C2  GLL H   1     30.367  21.927  35.384  1.00 28.20      C
ATOM  2050  C3  GLL H   1     29.770  21.431  36.710  1.00 28.42      C
ATOM  2051  C4  GLL H   1     28.226  21.455  36.650  1.00 28.59      C
ATOM  2052  C5  GLL H   1     27.623  21.260  38.035  1.00 29.41      C
ATOM  2053  O6  GLL H   1     26.564  21.811  38.323  1.00 29.10      O
ATOM  2054  O7  GLL H   1     28.182  20.544  38.872  1.00 28.72      O
ATOM  2055  C8  GLL H   1     30.930  23.326  35.546  1.00 28.44      C
ATOM  2056  O9  GLL H   1     31.829  23.753  34.734  1.00 28.04      O
ATOM  2057  O10 GLL H   1     30.504  24.085  36.478  1.00 29.50      O
ATOM  2107  OH2 WAT S   1     28.597  26.858  34.170  1.00 35.33      O
ATOM  2108  OH2 WAT S   2     39.874  15.622  52.951  1.00 27.02      O
ATOM  2109  OH2 WAT S   3     47.806  29.582  41.793  1.00 26.82      O
ATOM  2110  OH2 WAT S   4     32.712  12.071  49.955  1.00 33.48      O
ATOM  2111  OH2 WAT S   5     34.388  29.141  28.290  1.00 23.66      O
ATOM  2112  OH2 WAT S   6     29.860  12.057  36.929  1.00 28.75      O
ATOM  2113  OH2 WAT S   7     18.596  31.078  31.314  1.00 34.56      O
ATOM  2114  OH2 WAT S   8     43.746  30.135  36.454  1.00 31.70      O
ATOM  2115  OH2 WAT S   9     40.710  28.228  24.786  1.00 32.34      O
ATOM  2116  OH2 WAT S  10     40.249  20.233  54.144  1.00 31.31      O
ATOM  2117  OH2 WAT S  11     50.729  22.205  49.175  1.00 29.78      O
ATOM  2118  OH2 WAT S  12     36.244  25.185  28.517  1.00 31.80      O
ATOM  2119  OH2 WAT S  13     29.586   1.690  31.020  1.00 35.67      O
ATOM  2120  OH2 WAT S  14     27.347   8.426  41.609  1.00 33.85      O
ATOM  2121  OH2 WAT S  15     37.753  30.653  48.262  1.00 31.49      O
ATOM  2122  OH2 WAT S  16     39.852   0.508  38.143  1.00 34.51      O
ATOM  2123  OH2 WAT S  17     49.787  10.549  30.555  1.00 37.19      O
ATOM  2124  OH2 WAT S  18     48.590  27.775  45.618  1.00 37.05      O
ATOM  2125  OH2 WAT S  19     46.426  30.341  36.837  1.00 31.78      O
ATOM  2126  OH2 WAT S  20     26.420  26.789  43.445  1.00 49.61      O
ATOM  2127  OH2 WAT S  21     46.268  30.739  29.048  1.00 36.68      O
ATOM  2128  OH2 WAT S  22     51.867  28.804  43.136  1.00 49.35      O
ATOM  2129  OH2 WAT S  23     36.825  15.509  25.141  1.00 33.48      O
ATOM  2130  OH2 WAT S  24     33.895  12.303  25.137  1.00 32.90      O
ATOM  2131  OH2 WAT S  25     36.781  35.492  29.625  1.00 32.04      O
ATOM  2132  OH2 WAT S  26     33.992  25.683  29.926  1.00 34.00      O
ATOM  2133  OH2 WAT S  27     24.645  23.077  49.434  1.00 37.03      O
ATOM  2134  OH2 WAT S  28     37.658  21.847  53.629  1.00 28.23      O
ATOM  2135  OH2 WAT S  29     43.589  10.679  50.593  1.00 35.31      O
ATOM  2136  OH2 WAT S  30     23.719  24.494  52.323  1.00 35.79      O
ATOM  2137  OH2 WAT S  31     39.337  10.396  24.048  1.00 52.48      O
ATOM  2138  OH2 WAT S  32     30.718  16.193  20.614  1.00 43.40      O
ATOM  2139  OH2 WAT S  33     54.666   8.115  42.921  1.00 47.38      O
ATOM  2140  OH2 WAT S  34     31.589  30.437  35.873  1.00 47.91      O
ATOM  2141  OH2 WAT S  35     50.340  32.089  31.165  1.00 41.42      O
ATOM  2142  OH2 WAT S  36     52.796  22.874  51.515  1.00 43.37      O
ATOM  2143  OH2 WAT S  37     55.373  22.792  30.536  1.00 57.15      O
ATOM  2144  OH2 WAT S  38     39.463  35.817  35.231  1.00 32.47      O
ATOM  2145  OH2 WAT S  39     16.092  27.159  27.724  1.00 37.21      O
ATOM  2146  OH2 WAT S  40     25.640  24.780  14.005  1.00 45.10      O
ATOM  2147  OH2 WAT S  41     50.761   2.536  38.098  1.00 52.36      O
ATOM  2148  OH2 WAT S  42     18.634  34.668  30.052  1.00 43.13      O
ATOM  2149  OH2 WAT S  43     38.535  -2.076  28.925  1.00 32.09      O
ATOM  2150  OH2 WAT S  44     13.196  24.012  19.544  1.00 39.80      O
ATOM  2151  OH2 WAT S  45     31.357  26.426  13.729  1.00 42.37      O
```

Figure 8LL

```
ATOM  2152 OH2 WAT S  46     52.281  28.184  27.760  1.00 36.04           O
ATOM  2153 OH2 WAT S  47     46.418  33.201  38.411  1.00 44.49           O
ATOM  2154 OH2 WAT S  48     53.339  19.767  45.907  1.00 33.06           O
ATOM  2155 OH2 WAT S  49     46.967  16.612  52.076  1.00 30.83           O
ATOM  2156 OH2 WAT S  50     36.971  22.531  27.836  1.00 27.70           O
ATOM  2157 OH2 WAT S  51     34.404  33.315  13.713  1.00 63.94           O
ATOM  2158 OH2 WAT S  52     25.500  12.910  42.366  1.00 44.85           O
ATOM  2159 OH2 WAT S  53     41.068  33.656  19.666  1.00 61.38           O
ATOM  2160 OH2 WAT S  54     47.085  26.379  21.851  1.00 40.28           O
ATOM  2161 OH2 WAT S  55     20.530  37.341  28.713  1.00 42.17           O
ATOM  2162 OH2 WAT S  56     45.303  21.686  23.767  1.00 31.71           O
ATOM  2163 OH2 WAT S  57     32.171   3.766  47.945  1.00 39.12           O
ATOM  2164 OH2 WAT S  58     29.040  34.613  43.652  1.00 54.88           O
ATOM  2165 OH2 WAT S  59     63.169  17.639  43.696  1.00 51.86           O
ATOM  2166 OH2 WAT S  60     17.466  39.005  16.986  1.00 43.71           O
ATOM  2167 OH2 WAT S  61     31.214   5.360  30.303  1.00 35.40           O
ATOM  2168 OH2 WAT S  62     32.083  34.301  14.884  1.00 43.78           O
ATOM  2169 OH2 WAT S  63     56.027  25.650  46.067  1.00 55.28           O
ATOM  2170 OH2 WAT S  64     49.021  30.852  29.187  1.00 36.47           O
ATOM  2171 OH2 WAT S  65     23.639  30.939  17.071  1.00 45.30           O
ATOM  2172 OH2 WAT S  66     37.468  39.280  36.056  1.00 51.85           O
ATOM  2173 OH2 WAT S  67     36.224  28.879  18.295  1.00 42.91           O
ATOM  2174 OH2 WAT S  68     24.175  22.019  37.073  1.00 26.31           O
ATOM  2175 OH2 WAT S  69     22.152  26.896  48.344  1.00 61.11           O
ATOM  2176 OH2 WAT S  70     48.970   6.753  46.837  1.00 48.46           O
ATOM  2177 OH2 WAT S  71     42.273  27.745  52.837  1.00 33.63           O
ATOM  2178 OH2 WAT S  72     53.543  28.612  47.788  1.00 36.22           O
ATOM  2179 OH2 WAT S  73      8.907  23.447  21.629  1.00 50.44           O
ATOM  2180 OH2 WAT S  74     34.479  41.295  17.726  1.00 40.28           O
ATOM  2181 OH2 WAT S  75     34.584  20.083  21.656  1.00 47.04           O
ATOM  2182 OH2 WAT S  76     48.365   7.218  39.795  1.00 37.47           O
ATOM  2183 OH2 WAT S  77     17.856  23.193  14.949  1.00 36.50           O
ATOM  2184 OH2 WAT S  78     22.607  24.686  38.024  1.00 40.25           O
ATOM  2185 OH2 WAT S  79     21.034  18.474  37.563  1.00 57.62           O
ATOM  2186 OH2 WAT S  80     52.538   9.289  46.345  1.00 43.42           O
ATOM  2187 OH2 WAT S  81     29.673  13.056  39.115  1.00 28.10           O
ATOM  2188 OH2 WAT S  82     25.423  30.052  47.729  1.00 43.44           O
ATOM  2189 OH2 WAT S  83     27.721  18.627  14.255  1.00 44.64           O
ATOM  2190 OH2 WAT S  84     59.509  32.103  35.721  1.00 63.08           O
ATOM  2191 OH2 WAT S  85     44.482  33.024  48.358  1.00 36.03           O
ATOM  2192 OH2 WAT S  86     41.973   7.788  49.345  1.00 50.35           O
ATOM  2193 OH2 WAT S  87     37.663  22.110  25.265  1.00 41.24           O
ATOM  2194 OH2 WAT S  88     25.957  12.097  36.912  1.00 36.00           O
ATOM  2195 OH2 WAT S  89     30.437  33.017  13.345  1.00 48.23           O
ATOM  2196 OH2 WAT S  90     37.438  31.243  38.851  1.00 49.55           O
ATOM  2197 OH2 WAT S  91     19.458  34.402  26.135  1.00 43.19           O
ATOM  2198 OH2 WAT S  92     58.475  14.110  43.025  1.00 52.43           O
ATOM  2199 OH2 WAT S  93     22.370  12.343  33.413  1.00 38.81           O
ATOM  2200 OH2 WAT S  94     40.451  32.550  14.618  1.00 58.82           O
ATOM  2201 OH2 WAT S  95     54.156  16.243  28.025  1.00 48.89           O
ATOM  2202 OH2 WAT S  96     12.252  20.214  20.621  1.00 44.94           O
ATOM  2203 OH2 WAT S  97     23.229  23.360  11.991  1.00 68.77           O
ATOM  2204 OH2 WAT S  98     13.653  34.410  21.575  1.00 50.48           O
ATOM  2205 OH2 WAT S  99     29.882  16.048  51.774  1.00 53.76           O
ATOM  2206 OH2 WAT S 100     34.851   9.916  49.548  1.00 36.26           O
ATOM  2207 OH2 WAT S 101     19.731  39.777  18.001  1.00 49.92           O
ATOM  2208 OH2 WAT S 102     32.811  27.414  53.799  1.00 52.41           O
ATOM  2209 OH2 WAT S 103     54.958  10.260  45.018  1.00 61.62           O
```

Figure 8MM

```
ATOM  2210 OH2 WAT S 104    26.795   8.100  24.207  1.00 39.76      O
ATOM  2211 OH2 WAT S 105    39.473  25.414  23.627  1.00 33.71      O
ATOM  2212 OH2 WAT S 106    42.444  29.282  22.951  1.00 55.44      O
ATOM  2213 OH2 WAT S 107    54.310   2.465  42.338  1.00 81.43      O
ATOM  2214 OH2 WAT S 108    32.145  22.002  57.937  1.00 69.67      O
ATOM  2215 OH2 WAT S 109    41.182  36.953  24.858  1.00 30.32      O
ATOM  2216 OH2 WAT S 110    51.408  18.218  47.152  1.00 39.60      O
ATOM  2217 OH2 WAT S 111    31.229  18.063  15.169  1.00 58.09      O
ATOM  2218 OH2 WAT S 112    47.275  32.201  26.136  1.00 75.84      O
ATOM  2219 OH2 WAT S 113    48.484  -3.729  34.355  1.00 49.03      O
ATOM  2220 OH2 WAT S 114    17.441  23.890  30.338  1.00 38.38      O
ATOM  2221 OH2 WAT S 115    23.853  34.456  13.715  1.00 61.47      O
ATOM  2222 OH2 WAT S 116    22.764  12.193  26.654  1.00 52.95      O
ATOM  2223 OH2 WAT S 117    23.980  15.802  45.364  1.00 50.14      O
ATOM  2224 OH2 WAT S 118    35.972  34.774  45.163  1.00 60.33      O
ATOM  2225 OH2 WAT S 119    37.807  19.398  24.708  1.00 61.62      O
ATOM  2226 OH2 WAT S 120    18.366  12.430  18.822  1.00 41.37      O
ATOM  2227 OH2 WAT S 121    28.690  28.104  42.174  1.00 64.02      O
ATOM  2228 OH2 WAT S 122    49.307   6.503  32.285  1.00 36.36      O
ATOM  2229 OH2 WAT S 123    43.722   4.110  29.378  1.00 44.89      O
ATOM  2230 OH2 WAT S 124    26.343  29.966   7.876  1.00 62.82      O
ATOM  2231 OH2 WAT S 125    16.563  15.951  28.970  1.00 51.98      O
ATOM  2232 OH2 WAT S 126    20.175  23.841  38.565  1.00 55.56      O
ATOM  2233 OH2 WAT S 127    20.576  26.542  40.567  1.00 46.61      O
ATOM  2234 OH2 WAT S 128    40.494  17.605  54.649  1.00 38.00      O
ATOM  2235 OH2 WAT S 129    32.794  26.121  16.217  1.00 40.24      O
ATOM  2236 OH2 WAT S 130    32.054  30.620  12.330  1.00 41.15      O
ATOM  2237 OH2 WAT S 131    24.132   9.866  33.561  1.00 38.41      O
ATOM  2238 OH2 WAT S 132    39.539  30.733  24.819  1.00 33.26      O
ATOM  2239 OH2 WAT S 133    29.283   9.374  37.492  1.00 32.82      O
ATOM  2240 OH2 WAT S 134    27.129  12.130  39.369  1.00 36.01      O
ATOM  2241 OH2 WAT S 135    16.237  13.797  27.208  1.00 39.89      O
ATOM  2242 OH2 WAT S 136    35.590  17.878  24.571  1.00 35.55      O
ATOM  2243 OH2 WAT S 137    22.902  19.820  36.431  1.00 38.01      O
ATOM  2244 OH2 WAT S 138    52.919  12.766  42.677  1.00 32.51      O
ATOM  2245 OH2 WAT S 139    30.240  31.220  40.494  1.00 52.62      O
ATOM  2246 OH2 WAT S 140    37.369  27.649  21.696  1.00 36.64      O
ATOM  2247 OH2 WAT S 141    42.712   1.260  30.209  1.00 50.21      O
ATOM  2248 OH2 WAT S 142    24.778   5.524  41.136  1.00 37.52      O
ATOM  2249 OH2 WAT S 143    49.022  30.149  44.178  1.00 39.81      O
ATOM  2250 OH2 WAT S 144    44.239  27.252  54.601  1.00 45.46      O
ATOM  2251 OH2 WAT S 145    34.188  24.808  21.734  1.00 47.86      O
ATOM  2252 OH2 WAT S 146    32.237  13.936  23.957  1.00 47.59      O
ATOM  2253 OH2 WAT S 147    24.826  31.905  13.806  1.00 57.46      O
ATOM  2254 OH2 WAT S 148    35.287  19.774  55.093  1.00 53.61      O
ATOM  2255 OH2 WAT S 149    37.524  19.283  55.693  1.00 45.09      O
ATOM  2256 OH2 WAT S 150    35.302   8.641  24.481  1.00 51.58      O
ATOM  2257 OH2 WAT S 151    59.678  21.694  39.012  1.00 57.80      O
ATOM  2258 OH2 WAT S 152    36.143  -0.978  27.333  1.00 48.54      O
ATOM  2259 OH2 WAT S 153    14.265  20.928  14.183  1.00 62.49      O
ATOM  2260 OH2 WAT S 154    23.418  29.667  49.908  1.00 54.71      O
ATOM  2261 OH2 WAT S 155    38.604  24.411  54.120  1.00 52.33      O
ATOM  2262 OH2 WAT S 156    27.339  19.921  12.078  1.00 61.52      O
ATOM  2263 OH2 WAT S 157    55.513  12.418  43.797  1.00 48.44      O
ATOM  2264 OH2 WAT S 158    41.570  30.546  53.130  1.00 44.74      O
ATOM  2265 OH2 WAT S 159    30.332   6.416  25.709  1.00 48.89      O
ATOM  2266 OH2 WAT S 160    39.099  33.676  39.711  1.00 61.97      O
ATOM  2267 OH2 WAT S 161    25.263   8.969  43.752  1.00 53.20      O
```

Figure 8NN

ATOM 2268 OH2 WAT S 162 38.420 33.913 42.190 1.00 50.80 O
ATOM 2269 OH2 WAT S 163 41.309 37.709 36.508 1.00 59.09 O
ATOM 2270 OH2 WAT S 164 39.795 36.567 20.290 1.00 53.69 O
ATOM 2271 OH2 WAT S 165 17.433 22.843 32.869 1.00 39.36 O
ATOM 2272 OH2 WAT S 166 37.147 1.819 26.855 1.00 35.01. O
ATOM 2273 OH2 WAT S 167 26.808 29.856 51.140 1.00 34.22 O
ATOM 2274 OH2 WAT S 168 20.735 23.758 11.662 1.00 55.01 O
ATOM 2275 OH2 WAT S 169 37.554 20.226 20.434 1.00 54.40 O
ATOM 2276 OH2 WAT S 170 36.378 37.998 37.846 1.00 58.07 O
ATOM 2277 OH2 WAT S 171 18.421 12.604 25.862 1.00 45.72 O
ATOM 2278 OH2 WAT S 172 51.494 14.522 49.973 1.00 41.63 O
ATOM 2279 OH2 WAT S 173 39.132 29.730 18.357 1.00 56.55 O
ATOM 2280 OH2 WAT S 174 45.973 38.322 32.563 1.00 51.66 O
ATOM 2281 OH2 WAT S 175 51.494 34.523 30.878 1.00 51.26 O
ATOM 2282 OH2 WAT S 176 56.959 19.644 38.366 1.00 45.11 O
ATOM 2283 OH2 WAT S 177 27.770 26.356 13.109 1.00 51.59 O
ATOM 2284 OH2 WAT S 178 39.887 26.852 53.281 1.00 46.00 O
ATOM 2285 OH2 WAT S 179 31.617 7.635 49.956 1.00 42.18 O
ATOM 2286 OH2 WAT S 180 43.461 14.656 22.788 1.00 53.80 O
ATOM 2287 OH2 WAT S 181 39.538 18.123 23.159 1.00 56.96 O
ATOM 2288 OH2 WAT S 182 36.797 22.058 22.239 1.00 50.84 O
ATOM 2289 OH2 WAT S 183 15.670 13.383 19.237 1.00 48.91 O
ATOM 2290 OH2 WAT S 184 40.886 32.074 51.060 1.00 46.64 O
ATOM 2291 OH2 WAT S 185 46.429 3.853 37.759 1.00 47.74 O
ATOM 2292 OH2 WAT S 186 51.828 28.947 45.746 1.00 49.80 O
ATOM 2293 OH2 WAT S 187 37.821 12.326 23.248 1.00 59.05 O
ATOM 2294 OH2 WAT S 188 41.682 4.205 47.107 1.00 54.60 O
ATOM 2295 OH2 WAT S 189 24.396 40.185 10.597 1.00 65.04 O
ATOM 2296 OH2 WAT S 190 60.922 7.799 33.813 1.00 57.91 O
ATOM 2297 OH2 WAT S 191 59.350 17.293 37.717 1.00 60.20 O
ATOM 2298 OH2 WAT S 192 26.261 35.674 43.488 1.00 58.18 O
ATOM 2299 OH2 WAT S 193 32.421 28.845 41.543 1.00 57.00 O
ATOM 2300 OH2 WAT S 194 15.680 35.028 23.064 1.00 64.42 O
ATOM 2301 OH2 WAT S 195 38.794 4.828 49.890 1.00 58.11 O
ATOM 2302 OH2 WAT S 196 31.824 29.606 54.893 1.00 42.20 O
ATOM 2303 OH2 WAT S 197 56.033 18.872 46.171 1.00 43.23 O
ATOM 2304 OH2 WAT S 198 9.962 19.461 22.243 1.00 51.63 O
ATOM 2305 OH2 WAT S 199 18.489 10.150 20.863 1.00 54.24 O
ATOM 2306 OH2 WAT S 200 33.066 12.917 52.359 1.00 57.46 O
ATOM 2307 OH2 WAT S 201 30.483 0.016 45.976 1.00 48.00 O
ATOM 2308 OH2 WAT S 202 24.662 11.625 21.208 1.00 44.16 O
ATOM 2309 OH2 WAT S 203 46.715 24.249 23.656 1.00 41.75 O
ATOM 2310 OH2 WAT S 204 17.418 39.478 23.453 1.00 59.60 O
ATOM 2311 OH2 WAT S 205 36.419 43.376 23.037 1.00 52.17 O
ATOM 2312 OH2 WAT S 206 34.959 24.297 19.008 1.00 56.28 O
ATOM 2313 OH2 WAT S 207 43.180 39.844 30.801 1.00 59.11 O
ATOM 2314 OH2 WAT S 208 42.011 9.023 23.239 1.00 63.89 O
ATOM 2315 OH2 WAT S 209 22.676 12.375 19.314 1.00 53.20 O
ATOM 2316 OH2 WAT S 210 17.558 10.038 24.521 1.00 61.87 O
ATOM 2317 OH2 WAT S 211 48.462 5.142 44.693 1.00 58.47 O
ATOM 2318 OH2 WAT S 212 52.898 16.855 49.469 1.00 50.86 O
ATOM 2319 OH2 WAT S 213 37.726 41.234 24.591 1.00 47.40 O
ATOM 2320 OH2 WAT S 214 35.306 2.409 51.472 1.00 56.00 O
ATOM 2321 OH2 WAT S 215 34.107 13.946 54.277 1.00 59.41 O
ATOM 2322 OH2 WAT S 216 39.426 39.934 35.092 1.00 57.35 O
ATOM 2323 OH2 WAT S 217 49.879 15.750 52.077 1.00 59.87 O
ATOM 2324 OH2 WAT S 218 26.673 9.696 22.177 1.00 55.44 O
ATOM 2325 OH2 WAT S 219 22.122 22.199 39.182 1.00 45.37 O

Figure 8OO

```
ATOM  2326  OH2 WAT S 220     44.174   7.424  25.089  1.00 54.13       O
ATOM  2327  OH2 WAT S 221     53.760   5.884  44.382  1.00 54.00       O
END
```

Figure 9A

```
REMARK coordinates from minimization and B-factor refinement
REMARK refinement resolution: 500.0 - 1.9 A
REMARK starting r= 0.2224 free_r= 0.2451
REMARK final   r= 0.2185 free_r= 0.2440
REMARK rmsd bonds= 0.006037  rmsd angles=  1.31354
REMARK B rmsd for bonded mainchain atoms=  0.696  target= 1.5
REMARK B rmsd for bonded sidechain atoms=  0.779  target= 2.0
REMARK B rmsd for angle mainchain atoms=  1.253  target= 2.0
REMARK B rmsd for angle sidechain atoms=  1.286  target= 2.5
REMARK target= mlf  final wa= 0.882454  final rweight=0.367395
REMARK cycles= 1 coordinate steps= 150 B-factor steps= 100
REMARK sg= C222(1) a= 83.05 b= 112.82 c= 74.12 alpha= 90 beta= 90 gamma= 90
REMARK topology file 1  : MSI_CNX_TOPPAR:protein.top
REMARK topology file 2  : gll.top
REMARK topology file 3  : MSI_CNX_TOPPAR:water.top
REMARK topology file 4  : MSI_CNX_TOPPAR:ion.top
REMARK topology file 5  : uma.top
REMARK parameter file 1  : MSI_CNX_TOPPAR:protein_rep.param
REMARK parameter file 2  : gll.par
REMARK parameter file 3  : MSI_CNX_TOPPAR:water_rep.param
REMARK parameter file 4  : MSI_CNX_TOPPAR:ion.param
REMARK parameter file 5  : uma.par
REMARK molecular structure file: automatic
REMARK input coordinates: cns8_reb.pdb
REMARK reflection file= ../../../mosflm_esrf/muri_trn_free_unique.fob
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.9
REMARK initial B-factor correction applied to fobs :
REMARK   B11=   3.991 B22=  -8.126 B33=   4.136
REMARK   B12=   0.000 B13=   0.000 B23=   0.000
REMARK B-factor correction applied to coordinate array B:  -0.648
REMARK bulk solvent: (Mask) density level= 0.373583 e/A^3, B-factor= 48.6342 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range:    27807 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):  1265 (  4.5 % )
REMARK number of reflections rejected:                          0 (  0.0 % )
REMARK total number of reflections used:                    26542 ( 95.5 % )
REMARK number of reflections in working set:                25198 ( 90.6 % )
REMARK number of reflections in test set:                    1344 (  4.8 % )
CRYST1  83.050  112.820  74.120  90.00  90.00  90.00 C 2 2 21
REMARK FILENAME="refine.pdb"
REMARK DATE:Dec-11-2002  01:22:55      created by user: kemitl
REMARK Written by CNX VERSION:2000
ATOM     1  CB  PRO A  20     59.140  10.232  37.959  1.00 42.27       C
ATOM     2  CG  PRO A  20     60.118   9.060  37.995  1.00 42.63       C
ATOM     3  C   PRO A  20     58.220  11.395  35.947  1.00 41.62       C
ATOM     4  O   PRO A  20     59.154  12.042  35.457  1.00 41.55       O
ATOM     5  N   PRO A  20     59.374   9.210  35.773  1.00 42.45       N
ATOM     6  CD  PRO A  20     60.587   8.879  36.540  1.00 42.74       C
ATOM     7  CA  PRO A  20     58.468  10.041  36.605  1.00 42.13       C
ATOM     8  N   ARG A  21     56.961  11.820  35.938  1.00 40.77       N
ATOM     9  CA  ARG A  21     56.586  13.100  35.341  1.00 39.90       C
ATOM    10  CB  ARG A  21     55.792  12.875  34.053  1.00 41.14       C
ATOM    11  CG  ARG A  21     55.782  11.436  33.550  1.00 43.27       C
ATOM    12  CD  ARG A  21     54.592  10.646  34.098  1.00 44.85       C
ATOM    13  NE  ARG A  21     54.310   9.479  33.264  1.00 46.30       N
ATOM    14  CZ  ARG A  21     53.249   8.687  33.392  1.00 46.83       C
```

Figure 9B

```
ATOM   15 NH1 ARG A 21    52.338  8.918 34.332 1.00 46.85      N
ATOM   16 NH2 ARG A 21    53.095  7.661 32.562 1.00 47.39      N
ATOM   17 C  ARG A 21    55.738 13.891 36.327 1.00 38.37      C
ATOM   18 O  ARG A 21    55.175 13.321 37.261 1.00 38.35      O
ATOM   19 N  PRO A 22    55.635 15.217 36.134 1.00 36.71      N
ATOM   20 CD PRO A 22    56.249 16.056 35.092 1.00 36.55      C
ATOM   21 CA PRO A 22    54.834 16.026 37.053 1.00 35.10      C
ATOM   22 CB PRO A 22    54.956 17.441 36.483 1.00 35.61      C
ATOM   23 CG PRO A 22    55.312 17.226 35.048 1.00 36.83      C
ATOM   24 C  PRO A 22    53.392 15.548 37.177 1.00 33.33      C
ATOM   25 O  PRO A 22    52.737 15.204 36.193 1.00 33.12      O
ATOM   26 N  THR A 23    52.926 15.513 38.416 1.00 31.31      N
ATOM   27 CA THR A 23    51.579 15.073 38.734 1.00 28.82      C
ATOM   28 CB THR A 23    51.528 14.500 40.165 1.00 28.86      C
ATOM   29 OG1 THR A 23    52.345 13.324 40.230 1.00 29.00      O
ATOM   30 CG2 THR A 23    50.096 14.159 40.556 1.00 27.97      C
ATOM   31 C  THR A 23    50.615 16.241 38.626 1.00 27.22      C
ATOM   32 O  THR A 23    50.767 17.256 39.307 1.00 26.28      O
ATOM   33 N  VAL A 24    49.622 16.090 37.760 1.00 26.19      N
ATOM   34 CA VAL A 24    48.623 17.123 37.564 1.00 25.17      C
ATOM   35 CB VAL A 24    48.654 17.655 36.116 1.00 25.46      C
ATOM   36 CG1 VAL A 24    47.488 18.596 35.879 1.00 25.44      C
ATOM   37 CG2 VAL A 24    49.976 18.377 35.867 1.00 25.54      C
ATOM   38 C  VAL A 24    47.222 16.617 37.870 1.00 24.64      C
ATOM   39 O  VAL A 24    46.786 15.593 37.344 1.00 24.53      O
ATOM   40 N  LEU A 25    46.525 17.350 38.728 1.00 23.92      N
ATOM   41 CA LEU A 25    45.163 17.004 39.093 1.00 23.77      C
ATOM   42 CB LEU A 25    44.910 17.283 40.579 1.00 23.48      C
ATOM   43 CG LEU A 25    43.437 17.288 41.007 1.00 24.15      C
ATOM   44 CD1 LEU A 25    42.844 15.882 40.865 1.00 23.60      C
ATOM   45 CD2 LEU A 25    43.322 17.779 42.455 1.00 24.84      C
ATOM   46 C  LEU A 25    44.189 17.840 38.279 1.00 23.16      C
ATOM   47 O  LEU A 25    44.368 19.048 38.143 1.00 22.71      O
ATOM   48 N  VAL A 26    43.177 17.183 37.723 1.00 23.08      N
ATOM   49 CA VAL A 26    42.122 17.867 36.991 1.00 22.84      C
ATOM   50 CB VAL A 26    42.017 17.396 35.525 1.00 23.04      C
ATOM   51 CG1 VAL A 26    40.884 18.138 34.832 1.00 22.64      C
ATOM   52 CG2 VAL A 26    43.346 17.665 34.788 1.00 22.73      C
ATOM   53 C  VAL A 26    40.852 17.482 37.764 1.00 23.16      C
ATOM   54 O  VAL A 26    40.520 16.295 37.876 1.00 23.27      O
ATOM   55 N  PHE A 27    40.172 18.485 38.315 1.00 22.82      N
ATOM   56 CA PHE A 27    38.967 18.277 39.117 1.00 23.33      C
ATOM   57 CB PHE A 27    39.168 18.865 40.518 1.00 23.65      C
ATOM   58 CG PHE A 27    37.902 18.924 41.340 1.00 24.66      C
ATOM   59 CD1 PHE A 27    37.456 17.805 42.042 1.00 24.66      C
ATOM   60 CD2 PHE A 27    37.125 20.078 41.360 1.00 24.42      C
ATOM   61 CE1 PHE A 27    36.253 17.834 42.748 1.00 24.95      C
ATOM   62 CE2 PHE A 27    35.917 20.119 42.063 1.00 24.93      C
ATOM   63 CZ PHE A 27    35.480 18.995 42.756 1.00 25.18      C
ATOM   64 C  PHE A 27    37.687 18.879 38.547 1.00 23.64      C
ATOM   65 O  PHE A 27    37.705 19.941 37.931 1.00 24.06      O
ATOM   66 N  ASP A 28    36.575 18.187 38.773 1.00 23.82      N
ATOM   67 CA ASP A 28    35.253 18.651 38.358 1.00 23.43      C
ATOM   68 CB ASP A 28    34.957 18.343 36.885 1.00 23.14      C
ATOM   69 CG ASP A 28    33.602 18.896 36.443 1.00 23.57      C
ATOM   70 OD1 ASP A 28    32.893 18.244 35.646 1.00 23.23      O
ATOM   71 OD2 ASP A 28    33.239 19.998 36.903 1.00 24.14      O
ATOM   72 C  ASP A 28    34.226 17.924 39.202 1.00 23.59      C
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Figure 9C

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ATOM    73  O   ASP A  28      34.540  16.928  39.856  1.00 23.62           O
ATOM    74  N   SER A  29      32.996  18.421  39.179  1.00 23.49           N
ATOM    75  CA  SER A  29      31.904  17.800  39.913  1.00 23.63           C
ATOM    76  CB  SER A  29      30.717  18.757  39.969  1.00 23.55           C
ATOM    77  OG  SER A  29      30.313  19.099  38.657  1.00 24.80           O
ATOM    78  C   SER A  29      31.500  16.508  39.186  1.00 23.67           C
ATOM    79  O   SER A  29      31.007  15.564  39.804  1.00 23.60           O
ATOM    80  N   GLY A  30      31.721  16.471  37.874  1.00 23.60           N
ATOM    81  CA  GLY A  30      31.377  15.294  37.096  1.00 23.98           C
ATOM    82  C   GLY A  30      32.306  15.003  35.934  1.00 23.76           C
ATOM    83  O   GLY A  30      33.529  14.975  36.099  1.00 24.03           O
ATOM    84  N   VAL A  31      31.737  14.799  34.747  1.00 23.50           N
ATOM    85  CA  VAL A  31      32.536  14.491  33.566  1.00 23.42           C
ATOM    86  CB  VAL A  31      31.753  13.579  32.565  1.00 24.04           C
ATOM    87  CG1 VAL A  31      31.393  12.253  33.231  1.00 24.26           C
ATOM    88  CG2 VAL A  31      30.484  14.277  32.079  1.00 24.22           C
ATOM    89  C   VAL A  31      33.054  15.712  32.792  1.00 23.39           C
ATOM    90  O   VAL A  31      33.948  15.576  31.960  1.00 22.93           O
ATOM    91  N   GLY A  32      32.503  16.892  33.062  1.00 23.03           N
ATOM    92  CA  GLY A  32      32.933  18.083  32.341  1.00 23.53           C
ATOM    93  C   GLY A  32      34.434  18.316  32.374  1.00 23.94           C
ATOM    94  O   GLY A  32      35.018  18.803  31.406  1.00 23.61           O
ATOM    95  N   GLY A  33      35.058  17.971  33.496  1.00 23.88           N
ATOM    96  CA  GLY A  33      36.492  18.149  33.641  1.00 24.00           C
ATOM    97  C   GLY A  33      37.272  17.468  32.537  1.00 24.04           C
ATOM    98  O   GLY A  33      38.347  17.921  32.174  1.00 24.11           O
ATOM    99  N   LEU A  34      36.720  16.389  31.990  1.00 24.29           N
ATOM   100  CA  LEU A  34      37.377  15.653  30.923  1.00 24.12           C
ATOM   101  CB  LEU A  34      36.586  14.384  30.589  1.00 24.26           C
ATOM   102  CG  LEU A  34      36.559  13.331  31.703  1.00 24.52           C
ATOM   103  CD1 LEU A  34      35.609  12.209  31.311  1.00 24.48           C
ATOM   104  CD2 LEU A  34      37.969  12.795  31.940  1.00 24.92           C
ATOM   105  C   LEU A  34      37.586  16.474  29.652  1.00 23.95           C
ATOM   106  O   LEU A  34      38.524  16.212  28.907  1.00 24.13           O
ATOM   107  N   SER A  35      36.729  17.461  29.394  1.00 23.76           N
ATOM   108  CA  SER A  35      36.916  18.270  28.191  1.00 24.21           C
ATOM   109  CB  SER A  35      35.694  19.159  27.909  1.00 23.45           C
ATOM   110  OG  SER A  35      35.531  20.175  28.886  1.00 23.98           O
ATOM   111  C   SER A  35      38.173  19.137  28.347  1.00 24.34           C
ATOM   112  O   SER A  35      38.910  19.357  27.383  1.00 24.46           O
ATOM   113  N   VAL A  36      38.416  19.611  29.564  1.00 24.57           N
ATOM   114  CA  VAL A  36      39.582  20.444  29.847  1.00 25.04           C
ATOM   115  CB  VAL A  36      39.445  21.160  31.211  1.00 25.08           C
ATOM   116  CG1 VAL A  36      40.682  22.024  31.482  1.00 25.12           C
ATOM   117  CG2 VAL A  36      38.188  22.020  31.212  1.00 25.41           C
ATOM   118  C   VAL A  36      40.824  19.572  29.863  1.00 25.61           C
ATOM   119  O   VAL A  36      41.869  19.935  29.313  1.00 25.10           O
ATOM   120  N   TYR A  37      40.704  18.407  30.494  1.00 26.15           N
ATOM   121  CA  TYR A  37      41.816  17.478  30.550  1.00 26.62           C
ATOM   122  CB  TYR A  37      41.427  16.236  31.367  1.00 26.04           C
ATOM   123  CG  TYR A  37      42.210  14.999  31.006  1.00 26.11           C
ATOM   124  CD1 TYR A  37      41.696  14.065  30.106  1.00 26.04           C
ATOM   125  CE1 TYR A  37      42.431  12.937  29.737  1.00 26.06           C
ATOM   126  CD2 TYR A  37      43.483  14.777  31.532  1.00 26.28           C
ATOM   127  CE2 TYR A  37      44.227  13.654  31.167  1.00 26.29           C
ATOM   128  CZ  TYR A  37      43.694  12.742  30.274  1.00 26.29           C
ATOM   129  OH  TYR A  37      44.414  11.627  29.922  1.00 26.91           O
ATOM   130  C   TYR A  37      42.243  17.072  29.139  1.00 27.35           C
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Figure 9D

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ATOM   131  O   TYR A  37      43.431  16.998  28.840  1.00 27.42           O
ATOM   132  N   ASP A  38      41.270  16.815  28.274  1.00 28.14           N
ATOM   133  CA  ASP A  38      41.554  16.403  26.906  1.00 29.79           C
ATOM   134  CB  ASP A  38      40.234  16.233  26.149  1.00 30.37           C
ATOM   135  CG  ASP A  38      40.355  15.321  24.945  1.00 31.87           C
ATOM   136  OD1 ASP A  38      41.285  14.487  24.904  1.00 32.39           O
ATOM   137  OD2 ASP A  38      39.495  15.427  24.039  1.00 32.89           O
ATOM   138  C   ASP A  38      42.472  17.411  26.200  1.00 30.27           C
ATOM   139  O   ASP A  38      43.406  17.018  25.500  1.00 30.51           O
ATOM   140  N   GLU A  39      42.213  18.702  26.399  1.00 30.88           N
ATOM   141  CA  GLU A  39      43.032  19.759  25.799  1.00 32.05           C
ATOM   142  CB  GLU A  39      42.367  21.123  25.992  1.00 32.93           C
ATOM   143  CG  GLU A  39      41.075  21.325  25.219  1.00 35.19           C
ATOM   144  CD  GLU A  39      41.310  21.703  23.766  1.00 36.77           C
ATOM   145  OE1 GLU A  39      40.316  21.968  23.056  1.00 38.63           O
ATOM   146  OE2 GLU A  39      42.481  21.743  23.333  1.00 37.13           O
ATOM   147  C   GLU A  39      44.417  19.786  26.447  1.00 32.29           C
ATOM   148  O   GLU A  39      45.435  19.941  25.772  1.00 31.60           O
ATOM   149  N   ILE A  40      44.454  19.640  27.765  1.00 32.60           N
ATOM   150  CA  ILE A  40      45.726  19.646  28.472  1.00 33.11           C
ATOM   151  CB  ILE A  40      45.517  19.585  29.998  1.00 32.73           C
ATOM   152  CG2 ILE A  40      46.867  19.494  30.709  1.00 32.95           C
ATOM   153  CG1 ILE A  40      44.750  20.824  30.468  1.00 32.28           C
ATOM   154  CD1 ILE A  40      44.401  20.809  31.947  1.00 32.55           C
ATOM   155  C   ILE A  40      46.623  18.486  28.040  1.00 33.95           C
ATOM   156  O   ILE A  40      47.806  18.688  27.753  1.00 33.92           O
ATOM   157  N   ARG A  41      46.072  17.275  27.982  1.00 34.92           N
ATOM   158  CA  ARG A  41      46.872  16.118  27.593  1.00 36.38           C
ATOM   159  CB  ARG A  41      46.114  14.805  27.815  1.00 36.95           C
ATOM   160  CG  ARG A  41      44.970  14.556  26.850  1.00 38.65           C
ATOM   161  CD  ARG A  41      44.714  13.060  26.676  1.00 40.05           C
ATOM   162  NE  ARG A  41      43.499  12.807  25.905  1.00 41.30           N
ATOM   163  CZ  ARG A  41      43.076  11.600  25.541  1.00 41.65           C
ATOM   164  NH1 ARG A  41      43.770  10.518  25.872  1.00 41.91           N
ATOM   165  NH2 ARG A  41      41.952  11.475  24.847  1.00 42.04           N
ATOM   166  C   ARG A  41      47.324  16.188  26.141  1.00 37.23           C
ATOM   167  O   ARG A  41      48.347  15.618  25.780  1.00 36.68           O
ATOM   168  N   HIS A  42      46.554  16.870  25.303  1.00 38.38           N
ATOM   169  CA  HIS A  42      46.935  16.990  23.905  1.00 39.98           C
ATOM   170  CB  HIS A  42      45.803  17.637  23.102  1.00 40.97           C
ATOM   171  CG  HIS A  42      46.096  17.757  21.640  1.00 42.48           C
ATOM   172  CD2 HIS A  42      45.580  17.104  20.571  1.00 43.17           C
ATOM   173  ND1 HIS A  42      47.032  18.634  21.137  1.00 43.19           N
ATOM   174  CE1 HIS A  42      47.080  18.519  19.821  1.00 43.48           C
ATOM   175  NE2 HIS A  42      46.208  17.597  19.452  1.00 43.37           N
ATOM   176  C   HIS A  42      48.207  17.836  23.822  1.00 40.26           C
ATOM   177  O   HIS A  42      49.053  17.625  22.955  1.00 40.52           O
ATOM   178  N   LEU A  43      48.341  18.783  24.747  1.00 40.38           N
ATOM   179  CA  LEU A  43      49.500  19.662  24.795  1.00 40.54           C
ATOM   180  CB  LEU A  43      49.087  21.020  25.372  1.00 40.84           C
ATOM   181  CG  LEU A  43      50.118  22.150  25.372  1.00 40.88           C
ATOM   182  CD1 LEU A  43      50.521  22.468  23.935  1.00 41.44           C
ATOM   183  CD2 LEU A  43      49.533  23.386  26.043  1.00 40.98           C
ATOM   184  C   LEU A  43      50.638  19.065  25.631  1.00 40.74           C
ATOM   185  O   LEU A  43      51.812  19.224  25.299  1.00 40.80           O
ATOM   186  N   LEU A  44      50.284  18.379  26.715  1.00 40.77           N
ATOM   187  CA  LEU A  44      51.263  17.759  27.615  1.00 40.94           C
ATOM   188  CB  LEU A  44      51.281  18.515  28.942  1.00 40.98           C
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Figure 9E

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ATOM   189 CG  LEU A 44     51.493  20.023  28.814  1.00 40.82      C
ATOM   190 CD1 LEU A 44     51.011  20.721  30.066  1.00 40.73      C
ATOM   191 CD2 LEU A 44     52.964  20.307  28.550  1.00 41.26      C
ATOM   192 C   LEU A 44     50.841  16.310  27.841  1.00 41.15      C
ATOM   193 O   LEU A 44     50.325  15.955  28.903  1.00 41.15      O
ATOM   194 N   PRO A 45     51.075  15.445  26.843  1.00 41.22      N
ATOM   195 CD  PRO A 45     51.677  15.806  25.545  1.00 41.47      C
ATOM   196 CA  PRO A 45     50.725  14.021  26.873  1.00 41.13      C
ATOM   197 CB  PRO A 45     50.900  13.604  25.413  1.00 41.22      C
ATOM   198 CG  PRO A 45     52.040  14.456  24.968  1.00 41.02      C
ATOM   199 C   PRO A 45     51.418  13.044  27.826  1.00 41.10      C
ATOM   200 O   PRO A 45     50.885  11.961  28.077  1.00 41.10      O
ATOM   201 N   ASP A 46     52.576  13.400  28.373  1.00 40.74      N
ATOM   202 CA  ASP A 46     53.280  12.454  29.240  1.00 40.25      C
ATOM   203 CB  ASP A 46     54.765  12.400  28.854  1.00 41.61      C
ATOM   204 CG  ASP A 46     54.974  12.058  27.391  1.00 43.12      C
ATOM   205 OD1 ASP A 46     54.498  10.985  26.956  1.00 43.83      O
ATOM   206 OD2 ASP A 46     55.618  12.863  26.676  1.00 44.38      O
ATOM   207 C   ASP A 46     53.176  12.666  30.749  1.00 38.90      C
ATOM   208 O   ASP A 46     53.812  11.941  31.511  1.00 39.20      O
ATOM   209 N   LEU A 47     52.381  13.636  31.185  1.00 36.81      N
ATOM   210 CA  LEU A 47     52.249  13.907  32.614  1.00 34.74      C
ATOM   211 CB  LEU A 47     51.450  15.194  32.833  1.00 34.94      C
ATOM   212 CG  LEU A 47     51.913  16.438  32.077  1.00 34.69      C
ATOM   213 CD1 LEU A 47     51.018  17.604  32.434  1.00 35.28      C
ATOM   214 CD2 LEU A 47     53.358  16.746  32.428  1.00 35.67      C
ATOM   215 C   LEU A 47     51.564  12.774  33.364  1.00 33.31      C
ATOM   216 O   LEU A 47     50.968  11.881  32.758  1.00 33.06      O
ATOM   217 N   HIS A 48     51.678  12.800  34.689  1.00 31.91      N
ATOM   218 CA  HIS A 48     51.013  11.808  35.530  1.00 30.54      C
ATOM   219 CB  HIS A 48     51.794  11.524  36.814  1.00 30.57      C
ATOM   220 CG  HIS A 48     51.017  10.729  37.822  1.00 30.87      C
ATOM   221 CD2 HIS A 48     50.251   9.620  37.685  1.00 30.97      C
ATOM   222 ND1 HIS A 48     50.986  11.050  39.163  1.00 31.68      N
ATOM   223 CE1 HIS A 48     50.236  10.173  39.808  1.00 31.33      C
ATOM   224 NE2 HIS A 48     49.778   9.295  38.933  1.00 31.22      N
ATOM   225 C   HIS A 48     49.704  12.490  35.900  1.00 29.55      C
ATOM   226 O   HIS A 48     49.668  13.331  36.802  1.00 29.03      O
ATOM   227 N   TYR A 49     48.641  12.139  35.194  1.00 28.24      N
ATOM   228 CA  TYR A 49     47.349  12.754  35.441  1.00 27.76      C
ATOM   229 CB  TYR A 49     46.555  12.878  34.135  1.00 28.09      C
ATOM   230 CG  TYR A 49     47.108  13.881  33.145  1.00 28.48      C
ATOM   231 CD1 TYR A 49     47.890  13.471  32.066  1.00 28.86      C
ATOM   232 CE1 TYR A 49     48.375  14.395  31.124  1.00 29.12      C
ATOM   233 CD2 TYR A 49     46.823  15.242  33.275  1.00 28.88      C
ATOM   234 CE2 TYR A 49     47.301  16.173  32.350  1.00 29.31      C
ATOM   235 CZ  TYR A 49     48.075  15.741  31.275  1.00 29.63      C
ATOM   236 OH  TYR A 49     48.527  16.665  30.353  1.00 29.75      O
ATOM   237 C   TYR A 49     46.477  12.040  36.463  1.00 27.00      C
ATOM   238 O   TYR A 49     46.433  10.808  36.533  1.00 26.57      O
ATOM   239 N   ILE A 50     45.791  12.844  37.259  1.00 25.98      N
ATOM   240 CA  ILE A 50     44.854  12.340  38.243  1.00 24.91      C
ATOM   241 CB  ILE A 50     45.259  12.705  39.682  1.00 24.96      C
ATOM   242 CG2 ILE A 50     44.167  12.253  40.654  1.00 23.79      C
ATOM   243 CG1 ILE A 50     46.598  12.054  40.041  1.00 24.11      C
ATOM   244 CD1 ILE A 50     47.213  12.622  41.313  1.00 24.92      C
ATOM   245 C   ILE A 50     43.560  13.071  37.933  1.00 24.67      C
ATOM   246 O   ILE A 50     43.536  14.305  37.900  1.00 24.39      O
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Figure 9F

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ATOM   247  N   TYR A  51      42.498  12.321  37.671  1.00 24.20           N
ATOM   248  CA  TYR A  51      41.205  12.933  37.413  1.00 24.34           C
ATOM   249  CB  TYR A  51      40.549  12.369  36.148  1.00 24.65           C
ATOM   250  CG  TYR A  51      39.285  13.123  35.766  1.00 25.11           C
ATOM   251  CD1 TYR A  51      38.018  12.626  36.076  1.00 25.28           C
ATOM   252  CE1 TYR A  51      36.860  13.369  35.793  1.00 25.75           C
ATOM   253  CD2 TYR A  51      39.366  14.376  35.157  1.00 25.76           C
ATOM   254  CE2 TYR A  51      38.220  15.122  34.867  1.00 25.82           C
ATOM   255  CZ  TYR A  51      36.974  14.620  35.189  1.00 26.04           C
ATOM   256  OH  TYR A  51      35.856  15.394  34.926  1.00 25.60           O
ATOM   257  C   TYR A  51      40.337  12.612  38.616  1.00 24.47           C
ATOM   258  O   TYR A  51      40.221  11.451  39.014  1.00 24.67           O
ATOM   259  N   ALA A  52      39.740  13.637  39.208  1.00 24.11           N
ATOM   260  CA  ALA A  52      38.878  13.425  40.363  1.00 23.89           C
ATOM   261  CB  ALA A  52      39.533  13.994  41.619  1.00 23.82           C
ATOM   262  C   ALA A  52      37.533  14.090  40.131  1.00 23.96           C
ATOM   263  O   ALA A  52      37.466  15.253  39.723  1.00 23.07           O
ATOM   264  N   PHE A  53      36.461  13.347  40.372  1.00 23.37           N
ATOM   265  CA  PHE A  53      35.132  13.906  40.208  1.00 23.51           C
ATOM   266  CB  PHE A  53      34.474  13.388  38.909  1.00 23.73           C
ATOM   267  CG  PHE A  53      34.310  11.889  38.838  1.00 24.04           C
ATOM   268  CD1 PHE A  53      33.054  11.309  39.007  1.00 23.82           C
ATOM   269  CD2 PHE A  53      35.398  11.066  38.559  1.00 24.45           C
ATOM   270  CE1 PHE A  53      32.882   9.929  38.895  1.00 24.38           C
ATOM   271  CE2 PHE A  53      35.242   9.679  38.445  1.00 24.39           C
ATOM   272  CZ  PHE A  53      33.978   9.111  38.614  1.00 24.35           C
ATOM   273  C   PHE A  53      34.276  13.625  41.444  1.00 23.79           C
ATOM   274  O   PHE A  53      34.305  12.528  42.013  1.00 22.86           O
ATOM   275  N   ASP A  54      33.533  14.642  41.868  1.00 23.79           N
ATOM   276  CA  ASP A  54      32.682  14.541  43.051  1.00 24.06           C
ATOM   277  CB  ASP A  54      32.563  15.916  43.714  1.00 23.89           C
ATOM   278  CG  ASP A  54      31.963  15.840  45.109  1.00 23.89           C
ATOM   279  OD1 ASP A  54      31.577  14.727  45.538  1.00 22.90           O
ATOM   280  OD2 ASP A  54      31.880  16.894  45.772  1.00 23.05           O
ATOM   281  C   ASP A  54      31.289  14.002  42.734  1.00 24.18           C
ATOM   282  O   ASP A  54      30.312  14.750  42.734  1.00 23.82           O
ATOM   283  N   ASN A  55      31.191  12.698  42.488  1.00 24.17           N
ATOM   284  CA  ASN A  55      29.905  12.103  42.170  1.00 25.09           C
ATOM   285  CB  ASN A  55      30.090  10.674  41.631  1.00 25.26           C
ATOM   286  CG  ASN A  55      30.731   9.737  42.639  1.00 25.36           C
ATOM   287  OD1 ASN A  55      31.791  10.028  43.201  1.00 24.79           O
ATOM   288  ND2 ASN A  55      30.092   8.592  42.864  1.00 25.74           N
ATOM   289  C   ASN A  55      28.970  12.110  43.376  1.00 25.56           C
ATOM   290  O   ASN A  55      27.770  11.915  43.226  1.00 25.79           O
ATOM   291  N   VAL A  56      29.520  12.362  44.561  1.00 25.66           N
ATOM   292  CA  VAL A  56      28.731  12.405  45.794  1.00 26.16           C
ATOM   293  CB  VAL A  56      29.642  12.231  47.043  1.00 26.47           C
ATOM   294  CG1 VAL A  56      28.888  12.614  48.320  1.00 26.82           C
ATOM   295  CG2 VAL A  56      30.112  10.785  47.140  1.00 26.75           C
ATOM   296  C   VAL A  56      27.930  13.704  45.950  1.00 26.34           C
ATOM   297  O   VAL A  56      26.779  13.683  46.395  1.00 26.27           O
ATOM   298  N   ALA A  57      28.528  14.831  45.576  1.00 25.69           N
ATOM   299  CA  ALA A  57      27.846  16.106  45.723  1.00 25.62           C
ATOM   300  CB  ALA A  57      28.721  17.072  46.509  1.00 25.61           C
ATOM   301  C   ALA A  57      27.399  16.740  44.405  1.00 25.80           C
ATOM   302  O   ALA A  57      26.813  17.820  44.406  1.00 25.99           O
ATOM   303  N   PHE A  58      27.675  16.079  43.284  1.00 25.66           N
ATOM   304  CA  PHE A  58      27.242  16.595  41.984  1.00 25.94           C
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Figure 9G

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ATOM   305  CB  PHE A  58      27.689  15.659  40.856  1.00 25.77           C
ATOM   306  CG  PHE A  58      27.101  16.006  39.517  1.00 26.33           C
ATOM   307  CD1 PHE A  58      27.725  16.933  38.684  1.00 26.01           C
ATOM   308  CD2 PHE A  58      25.892  15.445  39.112  1.00 26.14           C
ATOM   309  CE1 PHE A  58      27.152  17.300  37.467  1.00 26.79           C
ATOM   310  CE2 PHE A  58      25.308  15.807  37.893  1.00 27.07           C
ATOM   311  CZ  PHE A  58      25.938  16.735  37.071  1.00 27.22           C
ATOM   312  C   PHE A  58      25.714  16.601  42.045  1.00 26.23           C
ATOM   313  O   PHE A  58      25.123  15.651  42.555  1.00 26.27           O
ATOM   314  N   PRO A  59      25.053  17.645  41.507  1.00 26.87           N
ATOM   315  CD  PRO A  59      23.589  17.565  41.316  1.00 27.24           C
ATOM   316  CA  PRO A  59      25.591  18.836  40.838  1.00 27.09           C
ATOM   317  CB  PRO A  59      24.484  19.195  39.850  1.00 27.32           C
ATOM   318  CG  PRO A  59      23.257  18.898  40.647  1.00 27.45           C
ATOM   319  C   PRO A  59      25.902  19.993  41.788  1.00 27.44           C
ATOM   320  O   PRO A  59      25.197  20.214  42.776  1.00 26.87           O
ATOM   321  N   TYR A  60      26.968  20.725  41.476  1.00 28.08           N
ATOM   322  CA  TYR A  60      27.395  21.870  42.277  1.00 29.46           C
ATOM   323  CB  TYR A  60      28.873  22.182  41.988  1.00 28.52           C
ATOM   324  CG  TYR A  60      29.887  21.318  42.725  1.00 27.75           C
ATOM   325  CD1 TYR A  60      29.520  20.113  43.339  1.00 27.37           C
ATOM   326  CE1 TYR A  60      30.475  19.317  44.006  1.00 26.91           C
ATOM   327  CD2 TYR A  60      31.228  21.708  42.794  1.00 27.09           C
ATOM   328  CE2 TYR A  60      32.178  20.932  43.450  1.00 27.19           C
ATOM   329  CZ  TYR A  60      31.802  19.739  44.054  1.00 27.07           C
ATOM   330  OH  TYR A  60      32.758  18.982  44.698  1.00 25.80           O
ATOM   331  C   TYR A  60      26.539  23.119  41.991  1.00 30.92           C
ATOM   332  O   TYR A  60      26.389  23.993  42.849  1.00 30.67           O
ATOM   333  N   GLY A  61      25.981  23.190  40.785  1.00 33.00           N
ATOM   334  CA  GLY A  61      25.165  24.332  40.400  1.00 35.24           C
ATOM   335  C   GLY A  61      24.126  24.770  41.418  1.00 37.04           C
ATOM   336  O   GLY A  61      23.892  25.965  41.601  1.00 37.85           O
ATOM   337  N   GLU A  62      23.512  23.803  42.089  1.00 38.35           N
ATOM   338  CA  GLU A  62      22.479  24.069  43.088  1.00 39.52           C
ATOM   339  CB  GLU A  62      21.559  22.852  43.183  1.00 41.20           C
ATOM   340  CG  GLU A  62      22.340  21.562  43.450  1.00 43.11           C
ATOM   341  CD  GLU A  62      21.455  20.385  43.790  1.00 44.30           C
ATOM   342  OE1 GLU A  62      20.626  19.994  42.931  1.00 45.50           O
ATOM   343  OE2 GLU A  62      21.590  19.850  44.917  1.00 44.82           O
ATOM   344  C   GLU A  62      23.026  24.374  44.487  1.00 39.48           C
ATOM   345  O   GLU A  62      22.459  25.187  45.226  1.00 40.03           O
ATOM   346  N   LYS A  63      24.123  23.708  44.833  1.00 38.32           N
ATOM   347  CA  LYS A  63      24.772  23.827  46.135  1.00 37.54           C
ATOM   348  CB  LYS A  63      26.033  22.956  46.148  1.00 36.71           C
ATOM   349  CG  LYS A  63      25.795  21.494  45.761  1.00 36.22           C
ATOM   350  CD  LYS A  63      24.954  20.758  46.796  1.00 35.50           C
ATOM   351  CE  LYS A  63      24.888  19.257  46.509  1.00 34.57           C
ATOM   352  NZ  LYS A  63      24.287  18.933  45.180  1.00 33.47           N
ATOM   353  C   LYS A  63      25.130  25.233  46.623  1.00 37.13           C
ATOM   354  O   LYS A  63      25.354  26.153  45.833  1.00 37.17           O
ATOM   355  N   SER A  64      25.180  25.376  47.944  1.00 36.87           N
ATOM   356  CA  SER A  64      25.531  26.637  48.590  1.00 36.73           C
ATOM   357  CB  SER A  64      25.270  26.553  50.096  1.00 36.69           C
ATOM   358  OG  SER A  64      23.936  26.162  50.370  1.00 37.39           O
ATOM   359  C   SER A  64      27.017  26.869  48.360  1.00 36.81           C
ATOM   360  O   SER A  64      27.801  25.915  48.358  1.00 36.64           O
ATOM   361  N   GLU A  65      27.410  28.125  48.177  1.00 36.66           N
ATOM   362  CA  GLU A  65      28.813  28.439  47.947  1.00 36.97           C
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Figure 9H

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ATOM   363  CB  GLU A  65      28.985  29.926  47.611  1.00 38.23           C
ATOM   364  CG  GLU A  65      28.742  30.243  46.138  1.00 40.25           C
ATOM   365  CD  GLU A  65      28.841  31.730  45.815  1.00 42.02           C
ATOM   366  OE1 GLU A  65      29.763  32.403  46.336  1.00 43.02           O
ATOM   367  OE2 GLU A  65      28.006  32.223  45.023  1.00 43.06           O
ATOM   368  C   GLU A  65     29.702  28.050  49.122  1.00 36.16           C
ATOM   369  O   GLU A  65     30.831  27.606  48.917  1.00 36.24           O
ATOM   370  N   ALA A  66     29.198  28.202  50.345  1.00 35.06           N
ATOM   371  CA  ALA A  66      29.972  27.845  51.536  1.00 34.39           C
ATOM   372  CB  ALA A  66      29.191  28.190  52.794  1.00 34.26           C
ATOM   373  C   ALA A  66     30.317  26.348  51.522  1.00 33.80           C
ATOM   374  O   ALA A  66     31.420  25.943  51.903  1.00 33.49           O
ATOM   375  N   PHE A  67     29.367  25.528  51.087  1.00 32.84           N
ATOM   376  CA  PHE A  67      29.598  24.091  51.009  1.00 31.99           C
ATOM   377  CB  PHE A  67      28.308  23.339  50.657  1.00 31.83           C
ATOM   378  CG  PHE A  67      28.550  21.930  50.191  1.00 31.22           C
ATOM   379  CD1 PHE A  67      28.891  20.928  51.098  1.00 31.15           C
ATOM   380  CD2 PHE A  67      28.526  21.625  48.834  1.00 31.38           C
ATOM   381  CE1 PHE A  67      29.211  19.639  50.657  1.00 30.97           C
ATOM   382  CE2 PHE A  67      28.846  20.337  48.384  1.00 31.33           C
ATOM   383  CZ  PHE A  67      29.189  19.346  49.301  1.00 30.62           C
ATOM   384  C   PHE A  67     30.643  23.796  49.936  1.00 31.40           C
ATOM   385  O   PHE A  67     31.613  23.082  50.186  1.00 31.16           O
ATOM   386  N   ILE A  68     30.433  24.350  48.744  1.00 30.67           N
ATOM   387  CA  ILE A  68      31.338  24.139  47.618  1.00 30.11           C
ATOM   388  CB  ILE A  68      30.926  25.003  46.394  1.00 29.93           C
ATOM   389  CG2 ILE A  68      31.983  24.902  45.294  1.00 29.25           C
ATOM   390  CG1 ILE A  68      29.568  24.533  45.858  1.00 30.20           C
ATOM   391  CD1 ILE A  68      29.116  25.245  44.591  1.00 30.32           C
ATOM   392  C   ILE A  68     32.809  24.414  47.944  1.00 30.38           C
ATOM   393  O   ILE A  68     33.679  23.591  47.649  1.00 29.53           O
ATOM   394  N   VAL A  69     33.092  25.567  48.545  1.00 30.39           N
ATOM   395  CA  VAL A  69      34.470  25.907  48.886  1.00 30.68           C
ATOM   396  CB  VAL A  69      34.557  27.290  49.579  1.00 31.33           C
ATOM   397  CG1 VAL A  69      35.998  27.578  49.994  1.00 31.13           C
ATOM   398  CG2 VAL A  69      34.052  28.376  48.631  1.00 31.78           C
ATOM   399  C   VAL A  69     35.085  24.851  49.801  1.00 30.46           C
ATOM   400  O   VAL A  69     36.175  24.349  49.523  1.00 30.83           O
ATOM   401  N   GLU A  70     34.379  24.508  50.878  1.00 29.88           N
ATOM   402  CA  GLU A  70      34.869  23.518  51.834  1.00 30.07           C
ATOM   403  CB  GLU A  70      33.899  23.369  53.016  1.00 31.73           C
ATOM   404  CG  GLU A  70      33.763  24.597  53.925  1.00 35.37           C
ATOM   405  CD  GLU A  70      35.085  25.046  54.534  1.00 37.49           C
ATOM   406  OE1 GLU A  70      35.894  24.179  54.938  1.00 39.42           O
ATOM   407  OE2 GLU A  70      35.314  26.273  54.619  1.00 39.33           O
ATOM   408  C   GLU A  70     35.064  22.148  51.191  1.00 28.57           C
ATOM   409  O   GLU A  70     36.051  21.452  51.458  1.00 28.03           O
ATOM   410  N   ARG A  71     34.109  21.768  50.354  1.00 26.83           N
ATOM   411  CA  ARG A  71      34.140  20.478  49.677  1.00 25.52           C
ATOM   412  CB  ARG A  71      32.827  20.259  48.919  1.00 25.00           C
ATOM   413  CG  ARG A  71      32.717  18.924  48.195  1.00 24.55           C
ATOM   414  CD  ARG A  71      32.741  17.739  49.156  1.00 24.30           C
ATOM   415  NE  ARG A  71      32.481  16.490  48.437  1.00 24.43           N
ATOM   416  CZ  ARG A  71      32.569  15.278  48.973  1.00 24.76           C
ATOM   417  NH1 ARG A  71      32.915  15.130  50.248  1.00 24.34           N
ATOM   418  NH2 ARG A  71      32.321  14.210  48.227  1.00 24.54           N
ATOM   419  C   ARG A  71     35.320  20.345  48.722  1.00 24.66           C
ATOM   420  O   ARG A  71     36.044  19.352  48.769  1.00 24.09           O
```

Figure 9I

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ATOM   421  N   VAL A  72     35.521  21.342  47.863  1.00 23.70      N
ATOM   422  CA  VAL A  72     36.622  21.279  46.909  1.00 23.69      C
ATOM   423  CB  VAL A  72     36.537  22.428  45.883  1.00 23.55      C
ATOM   424  CG1 VAL A  72     37.697  22.337  44.904  1.00 23.48      C
ATOM   425  CG2 VAL A  72     35.206  22.337  45.125  1.00 24.07      C
ATOM   426  C   VAL A  72     37.976  21.301  47.623  1.00 23.44      C
ATOM   427  O   VAL A  72     38.907  20.607  47.216  1.00 23.28      O
ATOM   428  N   VAL A  73     38.085  22.088  48.686  1.00 23.43      N
ATOM   429  CA  VAL A  73     39.326  22.139  49.451  1.00 23.42      C
ATOM   430  CB  VAL A  73     39.264  23.209  50.571  1.00 24.16      C
ATOM   431  CG1 VAL A  73     40.438  23.033  51.540  1.00 24.47      C
ATOM   432  CG2 VAL A  73     39.316  24.604  49.964  1.00 24.03      C
ATOM   433  C   VAL A  73     39.578  20.755  50.076  1.00 23.35      C
ATOM   434  O   VAL A  73     40.707  20.277  50.094  1.00 23.23      O
ATOM   435  N   ALA A  74     38.527  20.108  50.575  1.00 22.61      N
ATOM   436  CA  ALA A  74     38.679  18.782  51.179  1.00 22.36      C
ATOM   437  CB  ALA A  74     37.382  18.355  51.870  1.00 22.18      C
ATOM   438  C   ALA A  74     39.085  17.736  50.132  1.00 22.47      C
ATOM   439  O   ALA A  74     39.916  16.867  50.400  1.00 21.70      O
ATOM   440  N   ILE A  75     38.499  17.806  48.940  1.00 22.12      N
ATOM   441  CA  ILE A  75     38.857  16.845  47.911  1.00 22.33      C
ATOM   442  CB  ILE A  75     37.898  16.942  46.695  1.00 22.09      C
ATOM   443  CG2 ILE A  75     38.439  16.106  45.531  1.00 21.64      C
ATOM   444  CG1 ILE A  75     36.502  16.455  47.107  1.00 22.35      C
ATOM   445  CD1 ILE A  75     35.414  16.664  46.055  1.00 21.88      C
ATOM   446  C   ILE A  75     40.319  17.017  47.460  1.00 22.41      C
ATOM   447  O   ILE A  75     41.038  16.033  47.306  1.00 22.76      O
ATOM   448  N   VAL A  76     40.770  18.253  47.259  1.00 22.98      N
ATOM   449  CA  VAL A  76     42.157  18.464  46.831  1.00 22.84      C
ATOM   450  CB  VAL A  76     42.436  19.945  46.478  1.00 23.18      C
ATOM   451  CG1 VAL A  76     43.922  20.122  46.125  1.00 23.17      C
ATOM   452  CG2 VAL A  76     41.557  20.376  45.294  1.00 22.52      C
ATOM   453  C   VAL A  76     43.106  18.030  47.951  1.00 23.01      C
ATOM   454  O   VAL A  76     44.206  17.542  47.706  1.00 22.66      O
ATOM   455  N   THR A  77     42.672  18.207  49.190  1.00 23.25      N
ATOM   456  CA  THR A  77     43.482  17.802  50.329  1.00 23.42      C
ATOM   457  CB  THR A  77     42.804  18.220  51.640  1.00 23.36      C
ATOM   458  OG1 THR A  77     42.715  19.650  51.672  1.00 23.52      O
ATOM   459  CG2 THR A  77     43.604  17.737  52.851  1.00 23.84      C
ATOM   460  C   THR A  77     43.673  16.285  50.305  1.00 23.65      C
ATOM   461  O   THR A  77     44.781  15.784  50.526  1.00 23.58      O
ATOM   462  N   ALA A  78     42.592  15.562  50.024  1.00 23.68      N
ATOM   463  CA  ALA A  78     42.635  14.104  49.973  1.00 24.18      C
ATOM   464  CB  ALA A  78     41.222  13.534  49.835  1.00 24.04      C
ATOM   465  C   ALA A  78     43.505  13.632  48.817  1.00 24.10      C
ATOM   466  O   ALA A  78     44.275  12.683  48.960  1.00 23.96      O
ATOM   467  N   VAL A  79     43.389  14.288  47.667  1.00 23.77      N
ATOM   468  CA  VAL A  79     44.206  13.892  46.533  1.00 24.22      C
ATOM   469  CB  VAL A  79     43.880  14.714  45.264  1.00 23.88      C
ATOM   470  CG1 VAL A  79     44.830  14.320  44.145  1.00 23.31      C
ATOM   471  CG2 VAL A  79     42.434  14.466  44.834  1.00 23.95      C
ATOM   472  C   VAL A  79     45.683  14.086  46.874  1.00 24.69      C
ATOM   473  O   VAL A  79     46.505  13.204  46.612  1.00 24.55      O
ATOM   474  N   GLN A  80     46.005  15.234  47.465  1.00 25.87      N
ATOM   475  CA  GLN A  80     47.381  15.560  47.847  1.00 27.88      C
ATOM   476  CB  GLN A  80     47.449  16.934  48.524  1.00 28.24      C
ATOM   477  CG  GLN A  80     48.853  17.292  49.006  1.00 29.92      C
ATOM   478  CD  GLN A  80     48.950  18.668  49.616  1.00 30.55      C
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Figure 9J

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ATOM   479 OE1 GLN A  80      48.356  18.943  50.662  1.00 32.95           O
ATOM   480 NE2 GLN A  80      49.703  19.546  48.971  1.00 31.00           N
ATOM   481 C   GLN A  80      47.991  14.521  48.781  1.00 29.34           C
ATOM   482 O   GLN A  80      49.211  14.361  48.833  1.00 28.95           O
ATOM   483 N   GLU A  81      47.143  13.824  49.527  1.00 30.79           N
ATOM   484 CA  GLU A  81      47.617  12.799  50.445  1.00 32.53           C
ATOM   485 CB  GLU A  81      46.525  12.443  51.453  1.00 34.55           C
ATOM   486 CG  GLU A  81      46.442  13.408  52.606  1.00 37.85           C
ATOM   487 CD  GLU A  81      47.735  13.457  53.399  1.00 39.61           C
ATOM   488 OE1 GLU A  81      48.230  12.381  53.806  1.00 41.29           O
ATOM   489 OE2 GLU A  81      48.258  14.569  53.618  1.00 41.33           O
ATOM   490 C   GLU A  81      48.035  11.559  49.675  1.00 32.42           C
ATOM   491 O   GLU A  81      48.974  10.865  50.066  1.00 32.74           O
ATOM   492 N   ARG A  82      47.337  11.285  48.578  1.00 31.81           N
ATOM   493 CA  ARG A  82      47.653  10.135  47.743  1.00 31.83           C
ATOM   494 CB  ARG A  82      46.456   9.777  46.852  1.00 32.76           C
ATOM   495 CG  ARG A  82      45.289   9.128  47.600  1.00 34.95           C
ATOM   496 CD  ARG A  82      45.701   7.773  48.180  1.00 36.27           C
ATOM   497 NE  ARG A  82      45.997   6.810  47.120  1.00 38.20           N
ATOM   498 CZ  ARG A  82      45.085   6.042  46.528  1.00 38.36           C
ATOM   499 NH1 ARG A  82      43.815   6.116  46.899  1.00 38.95           N
ATOM   500 NH2 ARG A  82      45.441   5.212  45.554  1.00 38.87           N
ATOM   501 C   ARG A  82      48.879  10.431  46.877  1.00 31.32           C
ATOM   502 O   ARG A  82      49.741   9.568  46.690  1.00 31.21           O
ATOM   503 N   TYR A  83      48.953  11.650  46.351  1.00 30.58           N
ATOM   504 CA  TYR A  83      50.079  12.057  45.510  1.00 30.30           C
ATOM   505 CB  TYR A  83      49.798  11.802  44.021  1.00 30.71           C
ATOM   506 CG  TYR A  83      49.710  10.362  43.580  1.00 31.39           C
ATOM   507 CD1 TYR A  83      48.481   9.717  43.484  1.00 31.23           C
ATOM   508 CE1 TYR A  83      48.394   8.404  43.034  1.00 32.06           C
ATOM   509 CD2 TYR A  83      50.857   9.655  43.218  1.00 31.62           C
ATOM   510 CE2 TYR A  83      50.780   8.342  42.767  1.00 32.08           C
ATOM   511 CZ  TYR A  83      49.550   7.724  42.677  1.00 32.19           C
ATOM   512 OH  TYR A  83      49.471   6.423  42.229  1.00 32.58           O
ATOM   513 C   TYR A  83      50.408  13.538  45.629  1.00 29.65           C
ATOM   514 O   TYR A  83      49.520  14.385  45.519  1.00 29.22           O
ATOM   515 N   PRO A  84      51.685  13.872  45.875  1.00 29.11           N
ATOM   516 CD  PRO A  84      52.799  13.019  46.335  1.00 29.50           C
ATOM   517 CA  PRO A  84      52.034  15.291  45.966  1.00 28.54           C
ATOM   518 CB  PRO A  84      53.539  15.257  46.206  1.00 29.05           C
ATOM   519 CG  PRO A  84      53.700  14.012  47.048  1.00 29.74           C
ATOM   520 C   PRO A  84      51.681  15.839  44.579  1.00 27.78           C
ATOM   521 O   PRO A  84      51.882  15.156  43.576  1.00 27.15           O
ATOM   522 N   LEU A  85      51.151  17.053  44.518  1.00 27.35           N
ATOM   523 CA  LEU A  85      50.741  17.626  43.239  1.00 26.90           C
ATOM   524 CB  LEU A  85      49.323  18.192  43.361  1.00 26.62           C
ATOM   525 CG  LEU A  85      48.230  17.259  43.889  1.00 26.34           C
ATOM   526 CD1 LEU A  85      46.923  18.030  44.073  1.00 26.18           C
ATOM   527 CD2 LEU A  85      48.049  16.102  42.926  1.00 26.09           C
ATOM   528 C   LEU A  85      51.661  18.725  42.731  1.00 26.93           C
ATOM   529 O   LEU A  85      52.148  19.540  43.501  1.00 26.47           O
ATOM   530 N   ALA A  86      51.908  18.731  41.428  1.00 27.16           N
ATOM   531 CA  ALA A  86      52.727  19.772  40.828  1.00 27.51           C
ATOM   532 CB  ALA A  86      53.411  19.244  39.560  1.00 27.79           C
ATOM   533 C   ALA A  86      51.775  20.922  40.484  1.00 27.57           C
ATOM   534 O   ALA A  86      52.149  22.091  40.512  1.00 28.41           O
ATOM   535 N   LEU A  87      50.524  20.581  40.189  1.00 27.71           N
ATOM   536 CA  LEU A  87      49.530  21.582  39.824  1.00 27.37           C
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Figure 9K

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ATOM   537  CB  LEU A  87      49.866  22.133  38.430  1.00 28.02           C
ATOM   538  CG  LEU A  87      48.916  23.067  37.676  1.00 27.98           C
ATOM   539  CD1 LEU A  87      49.721  23.825  36.624  1.00 28.10           C
ATOM   540  CD2 LEU A  87      47.788  22.274  37.013  1.00 28.31           C
ATOM   541  C   LEU A  87      48.134  20.972  39.817  1.00 27.07           C
ATOM   542  O   LEU A  87      47.973  19.779  39.558  1.00 27.09           O
ATOM   543  N   ALA A  88      47.132  21.797  40.101  1.00 26.70           N
ATOM   544  CA  ALA A  88      45.745  21.353  40.106  1.00 26.24           C
ATOM   545  CB  ALA A  88      45.218  21.285  41.528  1.00 26.54           C
ATOM   546  C   ALA A  88      44.876  22.299  39.282  1.00 26.33           C
ATOM   547  O   ALA A  88      45.040  23.522  39.326  1.00 25.93           O
ATOM   548  N   VAL A  89      43.949  21.719  38.532  1.00 26.38           N
ATOM   549  CA  VAL A  89      43.035  22.493  37.704  1.00 26.48           C
ATOM   550  CB  VAL A  89      43.100  22.057  36.225  1.00 26.98           C
ATOM   551  CG1 VAL A  89      42.184  22.945  35.388  1.00 26.51           C
ATOM   552  CG2 VAL A  89      44.535  22.111  35.719  1.00 26.37           C
ATOM   553  C   VAL A  89      41.605  22.285  38.174  1.00 26.45           C
ATOM   554  O   VAL A  89      41.128  21.153  38.248  1.00 26.61           O
ATOM   555  N   VAL A  90      40.930  23.375  38.513  1.00 26.03           N
ATOM   556  CA  VAL A  90      39.543  23.300  38.928  1.00 26.42           C
ATOM   557  CB  VAL A  90      39.195  24.432  39.916  1.00 26.37           C
ATOM   558  CG1 VAL A  90      37.744  24.315  40.361  1.00 26.82           C
ATOM   559  CG2 VAL A  90      40.123  24.355  41.137  1.00 26.76           C
ATOM   560  C   VAL A  90      38.787  23.490  37.615  1.00 26.74           C
ATOM   561  O   VAL A  90      38.371  24.601  37.288  1.00 26.48           O
ATOM   562  N   ALA A  91      38.657  22.405  36.853  1.00 26.82           N
ATOM   563  CA  ALA A  91      37.986  22.438  35.549  1.00 27.63           C
ATOM   564  CB  ALA A  91      38.468  21.276  34.694  1.00 27.04           C
ATOM   565  C   ALA A  91      36.488  22.356  35.758  1.00 28.11           C
ATOM   566  O   ALA A  91      35.820  21.459  35.242  1.00 27.96           O
ATOM   567  N   CYS A  92      35.979  23.327  36.509  1.00 29.18           N
ATOM   568  CA  CYS A  92      34.579  23.399  36.882  1.00 30.48           C
ATOM   569  CB  CYS A  92      34.402  22.573  38.163  1.00 30.27           C
ATOM   570  SG  CYS A  92      32.819  22.659  38.984  1.00 30.88           S
ATOM   571  C   CYS A  92      34.219  24.867  37.137  1.00 31.39           C
ATOM   572  O   CYS A  92      34.730  25.473  38.075  1.00 31.00           O
ATOM   573  N   ASN A  93      33.341  25.436  36.310  1.00 32.97           N
ATOM   574  CA  ASN A  93      32.937  26.837  36.470  1.00 34.50           C
ATOM   575  CB  ASN A  93      32.043  27.283  35.306  1.00 35.30           C
ATOM   576  CG  ASN A  93      32.770  27.298  33.982  1.00 36.40           C
ATOM   577  OD1 ASN A  93      32.983  26.251  33.360  1.00 37.59           O
ATOM   578  ND2 ASN A  93      33.165  28.489  33.539  1.00 36.95           N
ATOM   579  C   ASN A  93      32.218  27.128  37.784  1.00 35.02           C
ATOM   580  O   ASN A  93      32.473  28.151  38.426  1.00 35.62           O
ATOM   581  N   THR A  94      31.317  26.236  38.183  1.00 35.16           N
ATOM   582  CA  THR A  94      30.567  26.418  39.420  1.00 36.16           C
ATOM   583  CB  THR A  94      29.417  25.389  39.539  1.00 36.42           C
ATOM   584  OG1 THR A  94      29.934  24.063  39.353  1.00 36.99           O
ATOM   585  CG2 THR A  94      28.354  25.662  38.493  1.00 36.28           C
ATOM   586  C   THR A  94      31.436  26.311  40.668  1.00 36.39           C
ATOM   587  O   THR A  94      30.972  26.572  41.774  1.00 37.04           O
ATOM   588  N   ALA A  95      32.695  25.928  40.501  1.00 36.62           N
ATOM   589  CA  ALA A  95      33.587  25.803  41.654  1.00 37.07           C
ATOM   590  CB  ALA A  95      34.093  24.363  41.780  1.00 36.87           C
ATOM   591  C   ALA A  95      34.769  26.757  41.599  1.00 37.26           C
ATOM   592  O   ALA A  95      35.183  27.291  42.626  1.00 37.43           O
ATOM   593  N   SER A  96      35.304  26.978  40.405  1.00 37.85           N
ATOM   594  CA  SER A  96      36.464  27.844  40.245  1.00 38.98           C
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Figure 9L

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ATOM   595  CB  SER A  96      36.701  28.167  38.772  1.00 38.43           C
ATOM   596  OG  SER A  96      37.534  27.193  38.172  1.00 39.50           O
ATOM   597  C   SER A  96      36.403  29.140  41.031  1.00 39.55           C
ATOM   598  O   SER A  96      37.056  29.276  42.064  1.00 40.03           O
ATOM   599  N   THR A  97      35.621  30.090  40.540  1.00 40.03           N
ATOM   600  CA  THR A  97      35.507  31.386  41.193  1.00 40.80           C
ATOM   601  CB  THR A  97      34.206  32.086  40.782  1.00 41.54           C
ATOM   602  OG1 THR A  97      33.079  31.351  41.283  1.00 43.65           O
ATOM   603  CG2 THR A  97      34.116  32.152  39.266  1.00 42.47           C
ATOM   604  C   THR A  97      35.580  31.334  42.718  1.00 40.13           C
ATOM   605  O   THR A  97      36.587  31.730  43.322  1.00 40.25           O
ATOM   606  N   VAL A  98      34.524  30.819  43.333  1.00 38.98           N
ATOM   607  CA  VAL A  98      34.440  30.749  44.783  1.00 37.63           C
ATOM   608  CB  VAL A  98      33.074  30.183  45.210  1.00 38.05           C
ATOM   609  CG1 VAL A  98      31.951  31.032  44.616  1.00 37.94           C
ATOM   610  CG2 VAL A  98      32.949  28.735  44.752  1.00 37.58           C
ATOM   611  C   VAL A  98      35.521  29.956  45.520  1.00 36.84           C
ATOM   612  O   VAL A  98      35.789  30.230  46.689  1.00 36.41           O
ATOM   613  N   SER A  99      36.145  28.989  44.848  1.00 35.65           N
ATOM   614  CA  SER A  99      37.149  28.136  45.491  1.00 34.62           C
ATOM   615  CB  SER A  99      36.982  26.688  45.001  1.00 34.67           C
ATOM   616  OG  SER A  99      35.697  26.177  45.311  1.00 35.45           O
ATOM   617  C   SER A  99      38.626  28.504  45.353  1.00 33.65           C
ATOM   618  O   SER A  99      39.443  28.075  46.165  1.00 33.61           O
ATOM   619  N   LEU A 100      38.974  29.278  44.335  1.00 32.41           N
ATOM   620  CA  LEU A 100      40.371  29.635  44.103  1.00 31.86           C
ATOM   621  CB  LEU A 100      40.476  30.501  42.844  1.00 31.39           C
ATOM   622  CG  LEU A 100      40.052  29.816  41.538  1.00 31.77           C
ATOM   623  CD1 LEU A 100      40.345  30.741  40.359  1.00 31.20           C
ATOM   624  CD2 LEU A 100      40.813  28.498  41.363  1.00 31.65           C
ATOM   625  C   LEU A 100      41.131  30.286  45.272  1.00 31.53           C
ATOM   626  O   LEU A 100      42.227  29.851  45.620  1.00 31.21           O
ATOM   627  N   PRO A 101      40.570  31.336  45.887  1.00 31.41           N
ATOM   628  CD  PRO A 101      39.378  32.122  45.526  1.00 31.74           C
ATOM   629  CA  PRO A 101      41.289  31.958  47.006  1.00 31.39           C
ATOM   630  CB  PRO A 101      40.312  33.027  47.488  1.00 31.54           C
ATOM   631  CG  PRO A 101      39.657  33.455  46.202  1.00 31.94           C
ATOM   632  C   PRO A 101      41.642  30.960  48.111  1.00 31.01           C
ATOM   633  O   PRO A 101      42.784  30.908  48.574  1.00 30.97           O
ATOM   634  N   ALA A 102      40.657  30.168  48.522  1.00 30.66           N
ATOM   635  CA  ALA A 102      40.845  29.180  49.579  1.00 30.28           C
ATOM   636  CB  ALA A 102      39.507  28.531  49.927  1.00 30.65           C
ATOM   637  C   ALA A 102      41.867  28.110  49.210  1.00 29.99           C
ATOM   638  O   ALA A 102      42.675  27.692  50.049  1.00 29.77           O
ATOM   639  N   LEU A 103      41.833  27.668  47.957  1.00 29.36           N
ATOM   640  CA  LEU A 103      42.764  26.650  47.483  1.00 28.42           C
ATOM   641  CB  LEU A 103      42.322  26.126  46.119  1.00 27.97           C
ATOM   642  CG  LEU A 103      41.031  25.302  46.119  1.00 27.49           C
ATOM   643  CD1 LEU A 103      40.535  25.118  44.684  1.00 26.76           C
ATOM   644  CD2 LEU A 103      41.286  23.957  46.790  1.00 26.64           C
ATOM   645  C   LEU A 103      44.184  27.189  47.378  1.00 28.66           C
ATOM   646  O   LEU A 103      45.145  26.503  47.722  1.00 27.90           O
ATOM   647  N   ARG A 104      44.315  28.424  46.911  1.00 28.64           N
ATOM   648  CA  ARG A 104      45.630  29.021  46.761  1.00 29.38           C
ATOM   649  CB  ARG A 104      45.540  30.265  45.875  1.00 29.44           C
ATOM   650  CG  ARG A 104      45.362  29.904  44.407  1.00 30.55           C
ATOM   651  CD  ARG A 104      44.967  31.091  43.526  1.00 31.09           C
ATOM   652  NE  ARG A 104      44.866  30.655  42.134  1.00 31.83           N
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Figure 9M

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ATOM   653  CZ  ARG A 104      44.212  31.307  41.175  1.00 31.39           C
ATOM   654  NH1 ARG A 104      43.585  32.442  41.439  1.00 31.47           N
ATOM   655  NH2 ARG A 104      44.180  30.810  39.950  1.00 30.99           N
ATOM   656  C   ARG A 104      46.261  29.346  48.104  1.00 29.24           C
ATOM   657  O   ARG A 104      47.477  29.439  48.213  1.00 28.87           O
ATOM   658  N   GLU A 105      45.430  29.507  49.126  1.00 29.80           N
ATOM   659  CA  GLU A 105      45.928  29.791  50.465  1.00 31.03           C
ATOM   660  CB  GLU A 105      44.831  30.424  51.328  1.00 32.41           C
ATOM   661  CG  GLU A 105      45.138  30.405  52.827  1.00 34.95           C
ATOM   662  CD  GLU A 105      46.373  31.213  53.190  1.00 36.39           C
ATOM   663  OE1 GLU A 105      46.929  30.992  54.294  1.00 37.63           O
ATOM   664  OE2 GLU A 105      46.785  32.072  52.379  1.00 37.49           O
ATOM   665  C   GLU A 105      46.408  28.503  51.129  1.00 30.44           C
ATOM   666  O   GLU A 105      47.463  28.476  51.761  1.00 31.06           O
ATOM   667  N   LYS A 106      45.648  27.428  50.972  1.00 29.73           N
ATOM   668  CA  LYS A 106      46.023  26.175  51.605  1.00 29.26           C
ATOM   669  CB  LYS A 106      44.806  25.245  51.723  1.00 29.20           C
ATOM   670  CG  LYS A 106      45.091  24.005  52.595  1.00 29.25           C
ATOM   671  CD  LYS A 106      43.840  23.174  52.882  1.00 28.92           C
ATOM   672  CE  LYS A 106      44.150  22.010  53.840  1.00 28.67           C
ATOM   673  NZ  LYS A 106      42.965  21.124  54.082  1.00 28.66           N
ATOM   674  C   LYS A 106      47.168  25.410  50.943  1.00 29.05           C
ATOM   675  O   LYS A 106      47.993  24.806  51.635  1.00 28.51           O
ATOM   676  N   PHE A 107      47.240  25.445  49.617  1.00 28.37           N
ATOM   677  CA  PHE A 107      48.270  24.690  48.925  1.00 28.51           C
ATOM   678  CB  PHE A 107      47.627  23.857  47.815  1.00 28.11           C
ATOM   679  CG  PHE A 107      46.516  22.973  48.308  1.00 27.86           C
ATOM   680  CD1 PHE A 107      45.185  23.346  48.147  1.00 27.53           C
ATOM   681  CD2 PHE A 107      46.805  21.795  48.991  1.00 27.75           C
ATOM   682  CE1 PHE A 107      44.156  22.560  48.665  1.00 27.08           C
ATOM   683  CE2 PHE A 107      45.781  20.997  49.514  1.00 27.41           C
ATOM   684  CZ  PHE A 107      44.457  21.383  49.350  1.00 27.01           C
ATOM   685  C   PHE A 107      49.443  25.476  48.376  1.00 28.85           C
ATOM   686  O   PHE A 107      49.337  26.669  48.096  1.00 28.61           O
ATOM   687  N   ASP A 108      50.566  24.781  48.225  1.00 29.16           N
ATOM   688  CA  ASP A 108      51.781  25.394  47.716  1.00 29.72           C
ATOM   689  CB  ASP A 108      52.925  25.180  48.700  1.00 29.47           C
ATOM   690  CG  ASP A 108      52.721  25.959  49.973  1.00 29.74           C
ATOM   691  OD1 ASP A 108      52.567  27.196  49.880  1.00 29.19           O
ATOM   692  OD2 ASP A 108      52.700  25.344  51.058  1.00 29.72           O
ATOM   693  C   ASP A 108      52.163  24.914  46.333  1.00 29.83           C
ATOM   694  O   ASP A 108      53.335  24.699  46.018  1.00 30.36           O
ATOM   695  N   PHE A 109      51.145  24.724  45.511  1.00 29.48           N
ATOM   696  CA  PHE A 109      51.345  24.342  44.128  1.00 29.36           C
ATOM   697  CB  PHE A 109      51.079  22.844  43.895  1.00 28.81           C
ATOM   698  CG  PHE A 109      49.781  22.348  44.454  1.00 29.18           C
ATOM   699  CD1 PHE A 109      48.568  22.679  43.851  1.00 29.09           C
ATOM   700  CD2 PHE A 109      49.772  21.525  45.579  1.00 28.19           C
ATOM   701  CE1 PHE A 109      47.363  22.194  44.364  1.00 29.20           C
ATOM   702  CE2 PHE A 109      48.580  21.037  46.099  1.00 28.87           C
ATOM   703  CZ  PHE A 109      47.368  21.369  45.492  1.00 28.19           C
ATOM   704  C   PHE A 109      50.358  25.232  43.397  1.00 28.99           C
ATOM   705  O   PHE A 109      49.331  25.626  43.956  1.00 28.79           O
ATOM   706  N   PRO A 110      50.673  25.600  42.153  1.00 29.04           N
ATOM   707  CD  PRO A 110      51.823  25.213  41.318  1.00 28.89           C
ATOM   708  CA  PRO A 110      49.751  26.467  41.419  1.00 29.02           C
ATOM   709  CB  PRO A 110      50.515  26.761  40.128  1.00 28.79           C
ATOM   710  CG  PRO A 110      51.326  25.525  39.929  1.00 29.59           C
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Figure 9N

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ATOM   711  C   PRO A 110     48.381  25.839  41.182  1.00 28.61      C
ATOM   712  O   PRO A 110     48.259  24.630  40.990  1.00 28.77      O
ATOM   713  N   VAL A 111     47.352  26.673  41.224  1.00 28.61      N
ATOM   714  CA  VAL A 111     45.989  26.215  41.002  1.00 28.17      C
ATOM   715  CB  VAL A 111     45.101  26.457  42.240  1.00 27.94      C
ATOM   716  CG1 VAL A 111     43.683  25.945  41.978  1.00 26.91      C
ATOM   717  CG2 VAL A 111     45.710  25.759  43.467  1.00 27.23      C
ATOM   718  C   VAL A 111     45.417  26.987  39.822  1.00 28.51      C
ATOM   719  O   VAL A 111     45.482  28.213  39.786  1.00 28.55      O
ATOM   720  N   VAL A 112     44.871  26.263  38.854  1.00 28.78      N
ATOM   721  CA  VAL A 112     44.284  26.892  37.679  1.00 29.08      C
ATOM   722  CB  VAL A 112     44.691  26.145  36.387  1.00 29.31      C
ATOM   723  CG1 VAL A 112     43.996  26.753  35.175  1.00 29.34      C
ATOM   724  CG2 VAL A 112     46.185  26.215  36.213  1.00 28.86      C
ATOM   725  C   VAL A 112     42.772  26.891  37.810  1.00 29.49      C
ATOM   726  O   VAL A 112     42.175  25.895  38.227  1.00 29.47      O
ATOM   727  N   GLY A 113     42.160  28.021  37.475  1.00 29.33      N
ATOM   728  CA  GLY A 113     40.719  28.132  37.551  1.00 29.94      C
ATOM   729  C   GLY A 113     40.136  28.309  36.164  1.00 30.66      C
ATOM   730  O   GLY A 113     40.873  28.407  35.180  1.00 29.81      O
ATOM   731  N   VAL A 114     38.809  28.351  36.088  1.00 31.45      N
ATOM   732  CA  VAL A 114     38.121  28.518  34.811  1.00 32.36      C
ATOM   733  CB  VAL A 114     37.509  27.204  34.315  1.00 32.77      C
ATOM   734  CG1 VAL A 114     38.587  26.138  34.165  1.00 32.86      C
ATOM   735  CG2 VAL A 114     36.425  26.756  35.276  1.00 33.24      C
ATOM   736  C   VAL A 114     36.983  29.521  34.894  1.00 32.64      C
ATOM   737  O   VAL A 114     36.178  29.505  35.833  1.00 33.94      O
ATOM   738  N   VAL A 115     36.932  30.409  33.913  1.00 31.91      N
ATOM   739  CA  VAL A 115     35.869  31.395  33.830  1.00 31.47      C
ATOM   740  CB  VAL A 115     36.368  32.820  34.173  1.00 32.15      C
ATOM   741  CG1 VAL A 115     36.717  32.908  35.652  1.00 33.28      C
ATOM   742  CG2 VAL A 115     37.579  33.169  33.330  1.00 32.44      C
ATOM   743  C   VAL A 115     35.409  31.348  32.375  1.00 30.19      C
ATOM   744  O   VAL A 115     36.202  31.048  31.483  1.00 29.34      O
ATOM   745  N   PRO A 116     34.122  31.615  32.121  1.00 29.68      N
ATOM   746  CD  PRO A 116     33.044  31.894  33.088  1.00 29.83      C
ATOM   747  CA  PRO A 116     33.610  31.590  30.743  1.00 28.99      C
ATOM   748  CB  PRO A 116     32.195  32.141  30.894  1.00 29.53      C
ATOM   749  CG  PRO A 116     31.793  31.619  32.267  1.00 29.52      C
ATOM   750  C   PRO A 116     34.482  32.445  29.826  1.00 28.73      C
ATOM   751  O   PRO A 116     34.865  33.560  30.194  1.00 28.39      O
ATOM   752  N   ALA A 117     34.786  31.921  28.639  1.00 27.82      N
ATOM   753  CA  ALA A 117     35.638  32.607  27.663  1.00 28.21      C
ATOM   754  CB  ALA A 117     36.125  31.607  26.614  1.00 26.94      C
ATOM   755  C   ALA A 117     34.977  33.800  26.974  1.00 28.60      C
ATOM   756  O   ALA A 117     35.023  33.930  25.747  1.00 28.59      O
ATOM   757  N   ILE A 118     34.376  34.676  27.766  1.00 28.96      N
ATOM   758  CA  ILE A 118     33.710  35.848  27.225  1.00 29.91      C
ATOM   759  CB  ILE A 118     32.962  36.606  28.335  1.00 31.06      C
ATOM   760  CG2 ILE A 118     32.449  37.950  27.808  1.00 31.44      C
ATOM   761  CG1 ILE A 118     31.809  35.736  28.844  1.00 31.63      C
ATOM   762  CD1 ILE A 118     31.091  36.303  30.038  1.00 33.47      C
ATOM   763  C   ILE A 118     34.673  36.800  26.537  1.00 30.04      C
ATOM   764  O   ILE A 118     34.367  37.329  25.466  1.00 29.91      O
ATOM   765  N   LYS A 119     35.840  37.008  27.143  1.00 29.81      N
ATOM   766  CA  LYS A 119     36.836  37.915  26.584  1.00 30.04      C
ATOM   767  CB  LYS A 119     38.091  37.933  27.468  1.00 30.22      C
ATOM   768  CG  LYS A 119     39.130  38.955  27.020  1.00 30.96      C
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Figure 9O

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ATOM   769  CD  LYS A 119     40.292  39.050  27.988  1.00 31.45      C
ATOM   770  CE  LYS A 119     41.314  40.048  27.492  1.00 31.36      C
ATOM   771  NZ  LYS A 119     42.566  39.971  28.280  1.00 32.08      N
ATOM   772  C   LYS A 119     37.210  37.606  25.125  1.00 30.26      C
ATOM   773  O   LYS A 119     37.081  38.468  24.260  1.00 30.43      O
ATOM   774  N   PRO A 120     37.687  36.385  24.829  1.00 30.32      N
ATOM   775  CD  PRO A 120     38.119  35.261  25.679  1.00 30.42      C
ATOM   776  CA  PRO A 120     38.024  36.135  23.424  1.00 30.77      C
ATOM   777  CB  PRO A 120     38.743  34.782  23.469  1.00 30.78      C
ATOM   778  CG  PRO A 120     38.175  34.123  24.687  1.00 30.65      C
ATOM   779  C   PRO A 120     36.805  36.124  22.501  1.00 31.13      C
ATOM   780  O   PRO A 120     36.900  36.515  21.339  1.00 31.33      O
ATOM   781  N   ALA A 121     35.662  35.684  23.018  1.00 31.38      N
ATOM   782  CA  ALA A 121     34.447  35.632  22.214  1.00 31.88      C
ATOM   783  CB  ALA A 121     33.317  35.001  23.007  1.00 31.22      C
ATOM   784  C   ALA A 121     34.049  37.030  21.754  1.00 32.64      C
ATOM   785  O   ALA A 121     33.558  37.206  20.637  1.00 32.09      O
ATOM   786  N   ALA A 122     34.268  38.019  22.618  1.00 33.55      N
ATOM   787  CA  ALA A 122     33.931  39.405  22.305  1.00 34.91      C
ATOM   788  CB  ALA A 122     34.108  40.281  23.544  1.00 34.63      C
ATOM   789  C   ALA A 122     34.779  39.944  21.159  1.00 35.90      C
ATOM   790  O   ALA A 122     34.334  40.809  20.408  1.00 36.06      O
ATOM   791  N   ARG A 123     36.000  39.435  21.029  1.00 37.08      N
ATOM   792  CA  ARG A 123     36.901  39.866  19.962  1.00 38.64      C
ATOM   793  CB  ARG A 123     38.363  39.696  20.382  1.00 39.68      C
ATOM   794  CG  ARG A 123     38.775  40.468  21.618  1.00 41.76      C
ATOM   795  CD  ARG A 123     40.279  40.379  21.811  1.00 43.75      C
ATOM   796  NE  ARG A 123     41.000  40.999  20.701  1.00 45.71      N
ATOM   797  CZ  ARG A 123     42.320  40.959  20.547  1.00 46.46      C
ATOM   798  NH1 ARG A 123     43.071  40.321  21.435  1.00 47.45      N
ATOM   799  NH2 ARG A 123     42.891  41.564  19.512  1.00 47.03      N
ATOM   800  C   ARG A 123     36.689  39.068  18.678  1.00 39.10      C
ATOM   801  O   ARG A 123     37.252  39.405  17.636  1.00 39.34      O
ATOM   802  N   LEU A 124     35.886  38.011  18.749  1.00 39.13      N
ATOM   803  CA  LEU A 124     35.653  37.165  17.583  1.00 39.56      C
ATOM   804  CB  LEU A 124     35.776  35.686  17.975  1.00 39.49      C
ATOM   805  CG  LEU A 124     37.133  35.224  18.517  1.00 39.90      C
ATOM   806  CD1 LEU A 124     37.039  33.765  18.952  1.00 40.24      C
ATOM   807  CD2 LEU A 124     38.210  35.398  17.455  1.00 40.03      C
ATOM   808  C   LEU A 124     34.315  37.391  16.895  1.00 39.81      C
ATOM   809  O   LEU A 124     34.197  37.192  15.685  1.00 39.83      O
ATOM   810  N   THR A 125     33.311  37.807  17.659  1.00 39.86      N
ATOM   811  CA  THR A 125     31.991  38.027  17.096  1.00 40.44      C
ATOM   812  CB  THR A 125     30.981  38.482  18.179  1.00 40.32      C
ATOM   813  OG1 THR A 125     29.685  38.636  17.589  1.00 40.44      O
ATOM   814  CG2 THR A 125     31.411  39.803  18.809  1.00 40.44      C
ATOM   815  C   THR A 125     32.023  39.057  15.971  1.00 41.06      C
ATOM   816  O   THR A 125     32.777  40.028  16.022  1.00 40.79      O
ATOM   817  N   ALA A 126     31.206  38.826  14.949  1.00 41.50      N
ATOM   818  CA  ALA A 126     31.133  39.732  13.812  1.00 42.01      C
ATOM   819  CB  ALA A 126     31.214  38.943  12.507  1.00 41.90      C
ATOM   820  C   ALA A 126     29.837  40.532  13.861  1.00 42.35      C
ATOM   821  O   ALA A 126     29.798  41.685  13.427  1.00 42.99      O
ATOM   822  N   ASN A 127     28.778  39.928  14.394  1.00 41.88      N
ATOM   823  CA  ASN A 127     27.493  40.613  14.476  1.00 41.62      C
ATOM   824  CB  ASN A 127     26.350  39.641  14.147  1.00 41.84      C
ATOM   825  CG  ASN A 127     26.027  38.692  15.291  1.00 41.92      C
ATOM   826  OD1 ASN A 127     26.847  38.451  16.175  1.00 41.99      O
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Figure 9P

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ATOM   827 ND2 ASN A 127     24.822  38.135  15.264  1.00 41.74      N
ATOM   828 C   ASN A 127     27.266  41.262  15.834  1.00 41.10      C
ATOM   829 O   ASN A 127     26.241  41.902  16.066  1.00 41.43      O
ATOM   830 N   GLY A 128     28.234  41.101  16.730  1.00 40.81      N
ATOM   831 CA  GLY A 128     28.122  41.688  18.052  1.00 39.82      C
ATOM   832 C   GLY A 128     27.185  40.965  19.004  1.00 39.18      C
ATOM   833 O   GLY A 128     26.933  41.453  20.103  1.00 39.41      O
ATOM   834 N   ILE A 129     26.660  39.812  18.594  1.00 38.60      N
ATOM   835 CA  ILE A 129     25.757  39.044  19.451  1.00 37.56      C
ATOM   836 CB  ILE A 129     24.523  38.522  18.686  1.00 37.63      C
ATOM   837 CG2 ILE A 129     23.450  38.100  19.686  1.00 37.28      C
ATOM   838 CG1 ILE A 129     23.980  39.593  17.732  1.00 38.02      C
ATOM   839 CD1 ILE A 129     23.250  40.727  18.406  1.00 38.18      C
ATOM   840 C   ILE A 129     26.510  37.822  19.983  1.00 36.88      C
ATOM   841 O   ILE A 129     26.787  36.882  19.241  1.00 36.65      O
ATOM   842 N   VAL A 130     26.834  37.840  21.270  1.00 35.90      N
ATOM   843 CA  VAL A 130     27.554  36.733  21.877  1.00 34.41      C
ATOM   844 CB  VAL A 130     28.823  37.233  22.594  1.00 34.44      C
ATOM   845 CG1 VAL A 130     29.512  36.079  23.314  1.00 34.63      C
ATOM   846 CG2 VAL A 130     29.768  37.857  21.578  1.00 33.95      C
ATOM   847 C   VAL A 130     26.674  35.990  22.870  1.00 33.52      C
ATOM   848 O   VAL A 130     26.082  36.589  23.770  1.00 33.77      O
ATOM   849 N   GLY A 131     26.583  34.679  22.695  1.00 32.38      N
ATOM   850 CA  GLY A 131     25.779  33.877  23.593  1.00 31.20      C
ATOM   851 C   GLY A 131     26.626  33.212  24.667  1.00 30.54      C
ATOM   852 O   GLY A 131     27.799  32.903  24.453  1.00 29.56      O
ATOM   853 N   LEU A 132     26.032  33.009  25.837  1.00 29.94      N
ATOM   854 CA  LEU A 132     26.726  32.348  26.930  1.00 29.63      C
ATOM   855 CB  LEU A 132     26.970  33.314  28.094  1.00 29.35      C
ATOM   856 CG  LEU A 132     27.559  32.707  29.383  1.00 29.67      C
ATOM   857 CD1 LEU A 132     28.930  32.091  29.115  1.00 28.73      C
ATOM   858 CD2 LEU A 132     27.676  33.800  30.444  1.00 29.83      C
ATOM   859 C   LEU A 132     25.870  31.189  27.402  1.00 29.56      C
ATOM   860 O   LEU A 132     24.764  31.392  27.912  1.00 29.35      O
ATOM   861 N   LEU A 133     26.362  29.975  27.190  1.00 29.49      N
ATOM   862 CA  LEU A 133     25.658  28.776  27.632  1.00 30.26      C
ATOM   863 CB  LEU A 133     25.747  27.655  26.596  1.00 29.82      C
ATOM   864 CG  LEU A 133     24.832  27.685  25.382  1.00 29.97      C
ATOM   865 CD1 LEU A 133     25.087  26.431  24.561  1.00 29.36      C
ATOM   866 CD2 LEU A 133     23.370  27.738  25.831  1.00 29.56      C
ATOM   867 C   LEU A 133     26.374  28.328  28.891  1.00 30.96      C
ATOM   868 O   LEU A 133     27.577  28.064  28.867  1.00 30.93      O
ATOM   869 N   ALA A 134     25.641  28.258  29.991  1.00 31.95      N
ATOM   870 CA  ALA A 134     26.220  27.838  31.256  1.00 33.61      C
ATOM   871 CB  ALA A 134     26.671  29.056  32.057  1.00 33.35      C
ATOM   872 C   ALA A 134     25.157  27.080  32.022  1.00 34.73      C
ATOM   873 O   ALA A 134     24.021  26.963  31.567  1.00 34.36      O
ATOM   874 N   THR A 135     25.515  26.552  33.184  1.00 36.55      N
ATOM   875 CA  THR A 135     24.522  25.845  33.960  1.00 38.50      C
ATOM   876 CB  THR A 135     25.166  24.865  34.958  1.00 38.44      C
ATOM   877 OG1 THR A 135     24.136  24.057  35.544  1.00 38.63      O
ATOM   878 CG2 THR A 135     25.932  25.610  36.037  1.00 37.99      C
ATOM   879 C   THR A 135     23.676  26.890  34.683  1.00 40.21      C
ATOM   880 O   THR A 135     24.069  28.056  34.790  1.00 39.88      O
ATOM   881 N   ARG A 136     22.514  26.470  35.169  1.00 42.42      N
ATOM   882 CA  ARG A 136     21.592  27.374  35.840  1.00 44.95      C
ATOM   883 CB  ARG A 136     20.419  26.584  36.429  1.00 44.96      C
ATOM   884 CG  ARG A 136     19.310  27.468  36.958  1.00 45.04      C
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Figure 9Q

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ATOM    885  CD  ARG A 136      18.840  28.437  35.880  1.00 44.89           C
ATOM    886  NE  ARG A 136      18.043  29.521  36.442  1.00 45.05           N
ATOM    887  CZ  ARG A 136      17.561  30.538  35.736  1.00 44.74           C
ATOM    888  NH1 ARG A 136      17.794  30.611  34.433  1.00 44.68           N
ATOM    889  NH2 ARG A 136      16.854  31.484  36.337  1.00 44.28           N
ATOM    890  C   ARG A 136      22.226  28.242  36.921  1.00 46.64           C
ATOM    891  O   ARG A 136      21.963  29.443  36.987  1.00 46.85           O
ATOM    892  N   GLY A 137      23.064  27.637  37.759  1.00 48.47           N
ATOM    893  CA  GLY A 137      23.705  28.383  38.828  1.00 50.63           C
ATOM    894  C   GLY A 137      24.761  29.390  38.405  1.00 52.15           C
ATOM    895  O   GLY A 137      24.957  30.403  39.077  1.00 52.40           O
ATOM    896  N   THR A 138      25.439  29.122  37.295  1.00 53.81           N
ATOM    897  CA  THR A 138      26.493  30.007  36.804  1.00 55.54           C
ATOM    898  CB  THR A 138      27.342  29.297  35.732  1.00 55.54           C
ATOM    899  OG1 THR A 138      27.916  28.110  36.292  1.00 55.73           O
ATOM    900  CG2 THR A 138      28.458  30.209  35.236  1.00 55.51           C
ATOM    901  C   THR A 138      25.984  31.326  36.223  1.00 56.87           C
ATOM    902  O   THR A 138      26.685  32.337  36.264  1.00 57.03           O
ATOM    903  N   VAL A 139      24.769  31.314  35.682  1.00 58.47           N
ATOM    904  CA  VAL A 139      24.190  32.516  35.087  1.00 60.06           C
ATOM    905  CB  VAL A 139      23.136  32.151  34.009  1.00 59.85           C
ATOM    906  CG1 VAL A 139      23.805  31.438  32.846  1.00 59.91           C
ATOM    907  CG2 VAL A 139      22.055  31.273  34.613  1.00 59.77           C
ATOM    908  C   VAL A 139      23.537  33.432  36.123  1.00 61.27           C
ATOM    909  O   VAL A 139      23.011  34.495  35.783  1.00 61.39           O
ATOM    910  N   LYS A 140      23.581  33.020  37.386  1.00 62.64           N
ATOM    911  CA  LYS A 140      22.987  33.797  38.471  1.00 64.06           C
ATOM    912  CB  LYS A 140      22.045  32.902  39.285  1.00 64.35           C
ATOM    913  CG  LYS A 140      21.287  33.610  40.403  1.00 64.87           C
ATOM    914  CD  LYS A 140      20.275  32.679  41.073  1.00 65.20           C
ATOM    915  CE  LYS A 140      20.948  31.483  41.739  1.00 65.27           C
ATOM    916  NZ  LYS A 140      21.879  31.897  42.826  1.00 65.54           N
ATOM    917  C   LYS A 140      24.071  34.378  39.379  1.00 64.96           C
ATOM    918  O   LYS A 140      23.778  35.104  40.331  1.00 65.26           O
ATOM    919  N   ARG A 141      25.323  34.057  39.070  1.00 65.90           N
ATOM    920  CA  ARG A 141      26.464  34.523  39.850  1.00 66.86           C
ATOM    921  CB  ARG A 141      27.653  33.584  39.639  1.00 67.34           C
ATOM    922  CG  ARG A 141      27.501  32.230  40.306  1.00 68.13           C
ATOM    923  CD  ARG A 141      27.641  32.357  41.813  1.00 68.85           C
ATOM    924  NE  ARG A 141      27.467  31.079  42.497  1.00 69.48           N
ATOM    925  CZ  ARG A 141      26.332  30.387  42.510  1.00 69.74           C
ATOM    926  NH1 ARG A 141      25.263  30.847  41.873  1.00 69.96           N
ATOM    927  NH2 ARG A 141      26.262  29.238  43.167  1.00 69.94           N
ATOM    928  C   ARG A 141      26.889  35.946  39.511  1.00 67.23           C
ATOM    929  O   ARG A 141      26.868  36.353  38.349  1.00 67.16           O
ATOM    930  N   SER A 142      27.283  36.695  40.537  1.00 67.70           N
ATOM    931  CA  SER A 142      27.733  38.069  40.354  1.00 68.23           C
ATOM    932  CB  SER A 142      27.953  38.742  41.713  1.00 68.35           C
ATOM    933  OG  SER A 142      28.985  38.101  42.441  1.00 68.33           O
ATOM    934  C   SER A 142      29.040  38.061  39.567  1.00 68.56           C
ATOM    935  O   SER A 142      29.280  38.931  38.731  1.00 68.56           O
ATOM    936  N   TYR A 143      29.878  37.067  39.845  1.00 68.92           N
ATOM    937  CA  TYR A 143      31.164  36.921  39.171  1.00 69.28           C
ATOM    938  CB  TYR A 143      31.829  35.609  39.605  1.00 69.43           C
ATOM    939  CG  TYR A 143      33.270  35.440  39.157  1.00 69.75           C
ATOM    940  CD1 TYR A 143      33.605  35.365  37.804  1.00 69.92           C
ATOM    941  CE1 TYR A 143      34.930  35.193  37.395  1.00 69.93           C
ATOM    942  CD2 TYR A 143      34.300  35.339  40.094  1.00 69.94           C
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Figure 9R

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ATOM    943  CE2 TYR A 143      35.628  35.165  39.697  1.00 69.89           C
ATOM    944  CZ  TYR A 143      35.935  35.093  38.346  1.00 69.96           C
ATOM    945  OH  TYR A 143      37.243  34.918  37.950  1.00 69.93           O
ATOM    946  C   TYR A 143      30.945  36.916  37.659  1.00 69.53           C
ATOM    947  O   TYR A 143      31.741  37.474  36.900  1.00 69.51           O
ATOM    948  N   THR A 144      29.857  36.286  37.229  1.00 69.65           N
ATOM    949  CA  THR A 144      29.539  36.207  35.811  1.00 70.00           C
ATOM    950  CB  THR A 144      28.400  35.200  35.553  1.00 69.84           C
ATOM    951  OG1 THR A 144      28.718  33.944  36.168  1.00 69.88           O
ATOM    952  CG2 THR A 144      28.210  34.987  34.056  1.00 69.88           C
ATOM    953  C   THR A 144      29.123  37.577  35.277  1.00 70.22           C
ATOM    954  O   THR A 144      29.803  38.149  34.424  1.00 70.09           O
ATOM    955  N   HIS A 145      28.011  38.096  35.794  1.00 70.56           N
ATOM    956  CA  HIS A 145      27.484  39.395  35.378  1.00 70.96           C
ATOM    957  CB  HIS A 145      26.435  39.893  36.380  1.00 71.08           C
ATOM    958  CG  HIS A 145      25.333  38.916  36.643  1.00 71.36           C
ATOM    959  CD2 HIS A 145      24.826  38.435  37.803  1.00 71.32           C
ATOM    960  ND1 HIS A 145      24.602  38.327  35.633  1.00 71.38           N
ATOM    961  CE1 HIS A 145      23.694  37.525  36.160  1.00 71.57           C
ATOM    962  NE2 HIS A 145      23.809  37.572  37.475  1.00 71.52           N
ATOM    963  C   HIS A 145      28.582  40.446  35.245  1.00 71.08           C
ATOM    964  O   HIS A 145      28.543  41.296  34.354  1.00 71.07           O
ATOM    965  N   GLU A 146      29.559  40.381  36.142  1.00 71.21           N
ATOM    966  CA  GLU A 146      30.671  41.321  36.139  1.00 71.44           C
ATOM    967  CB  GLU A 146      31.480  41.165  37.428  1.00 71.84           C
ATOM    968  CG  GLU A 146      30.672  41.443  38.688  1.00 72.39           C
ATOM    969  CD  GLU A 146      31.393  41.024  39.956  1.00 72.71           C
ATOM    970  OE1 GLU A 146      30.792  41.143  41.043  1.00 73.01           O
ATOM    971  OE2 GLU A 146      32.558  40.576  39.868  1.00 72.85           O
ATOM    972  C   GLU A 146      31.575  41.116  34.930  1.00 71.35           C
ATOM    973  O   GLU A 146      31.878  42.063  34.206  1.00 71.49           O
ATOM    974  N   LEU A 147      32.004  39.876  34.714  1.00 71.27           N
ATOM    975  CA  LEU A 147      32.874  39.556  33.589  1.00 71.04           C
ATOM    976  CB  LEU A 147      33.146  38.050  33.546  1.00 71.09           C
ATOM    977  CG  LEU A 147      34.138  37.538  32.498  1.00 71.03           C
ATOM    978  CD1 LEU A 147      35.511  38.141  32.744  1.00 70.98           C
ATOM    979  CD2 LEU A 147      34.213  36.021  32.574  1.00 71.22           C
ATOM    980  C   LEU A 147      32.232  40.000  32.277  1.00 70.90           C
ATOM    981  O   LEU A 147      32.914  40.466  31.364  1.00 70.81           O
ATOM    982  N   ILE A 148      30.914  39.855  32.198  1.00 70.62           N
ATOM    983  CA  ILE A 148      30.163  40.233  31.008  1.00 70.53           C
ATOM    984  CB  ILE A 148      28.669  39.878  31.172  1.00 70.38           C
ATOM    985  CG2 ILE A 148      27.858  40.466  30.025  1.00 70.25           C
ATOM    986  CG1 ILE A 148      28.506  38.358  31.229  1.00 70.30           C
ATOM    987  CD1 ILE A 148      27.075  37.894  31.422  1.00 70.22           C
ATOM    988  C   ILE A 148      30.285  41.723  30.701  1.00 70.59           C
ATOM    989  O   ILE A 148      30.228  42.135  29.543  1.00 70.52           O
ATOM    990  N   ALA A 149      30.457  42.527  31.743  1.00 70.67           N
ATOM    991  CA  ALA A 149      30.579  43.967  31.573  1.00 70.58           C
ATOM    992  CB  ALA A 149      29.961  44.681  32.769  1.00 70.60           C
ATOM    993  C   ALA A 149      32.034  44.392  31.402  1.00 70.54           C
ATOM    994  O   ALA A 149      32.323  45.395  30.747  1.00 70.64           O
ATOM    995  N   ARG A 150      32.948  43.620  31.979  1.00 70.38           N
ATOM    996  CA  ARG A 150      34.370  43.938  31.906  1.00 70.26           C
ATOM    997  CB  ARG A 150      35.140  43.138  32.964  1.00 70.67           C
ATOM    998  CG  ARG A 150      36.625  43.473  33.034  1.00 71.26           C
ATOM    999  CD  ARG A 150      37.341  42.765  34.186  1.00 71.83           C
ATOM   1000  NE  ARG A 150      36.910  43.228  35.505  1.00 72.23           N
```

Figure 9S

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ATOM  1001  CZ  ARG A 150      35.813  42.811  36.134  1.00 72.55           C
ATOM  1002  NH1 ARG A 150      35.017  41.907  35.572  1.00 72.75           N
ATOM  1003  NH2 ARG A 150      35.511  43.299  37.331  1.00 72.57           N
ATOM  1004  C   ARG A 150      35.024  43.735  30.536  1.00 69.94           C
ATOM  1005  O   ARG A 150      35.754  44.611  30.063  1.00 69.86           O
ATOM  1006  N   PHE A 151      34.773  42.595  29.895  1.00 69.42           N
ATOM  1007  CA  PHE A 151      35.380  42.329  28.591  1.00 68.83           C
ATOM  1008  CB  PHE A 151      36.232  41.055  28.644  1.00 68.80           C
ATOM  1009  CG  PHE A 151      37.376  41.128  29.616  1.00 68.86           C
ATOM  1010  CD1 PHE A 151      37.245  40.621  30.905  1.00 68.95           C
ATOM  1011  CD2 PHE A 151      38.583  41.714  29.247  1.00 68.94           C
ATOM  1012  CE1 PHE A 151      38.302  40.696  31.813  1.00 68.85           C
ATOM  1013  CE2 PHE A 151      39.645  41.794  30.148  1.00 68.87           C
ATOM  1014  CZ  PHE A 151      39.503  41.284  31.432  1.00 68.86           C
ATOM  1015  C   PHE A 151      34.400  42.221  27.426  1.00 68.31           C
ATOM  1016  O   PHE A 151      34.789  41.836  26.324  1.00 68.27           O
ATOM  1017  N   ALA A 152      33.139  42.564  27.661  1.00 67.70           N
ATOM  1018  CA  ALA A 152      32.136  42.498  26.605  1.00 67.16           C
ATOM  1019  CB  ALA A 152      31.309  41.231  26.757  1.00 67.17           C
ATOM  1020  C   ALA A 152      31.229  43.725  26.621  1.00 66.73           C
ATOM  1021  O   ALA A 152      30.010  43.613  26.510  1.00 66.67           O
ATOM  1022  N   ASN A 153      31.838  44.899  26.751  1.00 66.39           N
ATOM  1023  CA  ASN A 153      31.098  46.156  26.791  1.00 65.89           C
ATOM  1024  CB  ASN A 153      31.966  47.243  27.436  1.00 66.36           C
ATOM  1025  CG  ASN A 153      31.191  48.517  27.732  1.00 66.81           C
ATOM  1026  OD1 ASN A 153      31.761  49.509  28.191  1.00 66.98           O
ATOM  1027  ND2 ASN A 153      29.886  48.495  27.478  1.00 66.94           N
ATOM  1028  C   ASN A 153      30.669  46.600  25.392  1.00 65.27           C
ATOM  1029  O   ASN A 153      29.718  47.364  25.237  1.00 65.39           O
ATOM  1030  N   GLU A 154      31.369  46.111  24.374  1.00 64.45           N
ATOM  1031  CA  GLU A 154      31.063  46.476  22.997  1.00 63.52           C
ATOM  1032  CB  GLU A 154      32.366  46.632  22.204  1.00 64.22           C
ATOM  1033  CG  GLU A 154      33.491  45.686  22.626  1.00 65.05           C
ATOM  1034  CD  GLU A 154      33.119  44.220  22.493  1.00 65.51           C
ATOM  1035  OE1 GLU A 154      32.757  43.794  21.373  1.00 65.78           O
ATOM  1036  OE2 GLU A 154      33.193  43.495  23.510  1.00 65.61           O
ATOM  1037  C   GLU A 154      30.121  45.519  22.269  1.00 62.47           C
ATOM  1038  O   GLU A 154      29.863  45.687  21.074  1.00 62.51           O
ATOM  1039  N   CYS A 155      29.602  44.522  22.981  1.00 60.87           N
ATOM  1040  CA  CYS A 155      28.684  43.561  22.373  1.00 59.19           C
ATOM  1041  CB  CYS A 155      29.437  42.294  21.950  1.00 59.45           C
ATOM  1042  SG  CYS A 155      30.164  41.355  23.315  1.00 59.76           S
ATOM  1043  C   CYS A 155      27.564  43.192  23.337  1.00 57.82           C
ATOM  1044  O   CYS A 155      27.679  43.403  24.541  1.00 57.62           O
ATOM  1045  N   GLN A 156      26.477  42.645  22.802  1.00 56.31           N
ATOM  1046  CA  GLN A 156      25.353  42.249  23.637  1.00 54.79           C
ATOM  1047  CB  GLN A 156      24.024  42.538  22.932  1.00 55.37           C
ATOM  1048  CG  GLN A 156      23.782  41.739  21.671  1.00 56.39           C
ATOM  1049  CD  GLN A 156      22.406  41.995  21.084  1.00 57.13           C
ATOM  1050  OE1 GLN A 156      22.079  43.123  20.703  1.00 57.59           O
ATOM  1051  NE2 GLN A 156      21.590  40.946  21.011  1.00 57.49           N
ATOM  1052  C   GLN A 156      25.457  40.767  23.976  1.00 53.29           C
ATOM  1053  O   GLN A 156      25.692  39.929  23.107  1.00 53.00           O
ATOM  1054  N   ILE A 157      25.275  40.453  25.252  1.00 51.67           N
ATOM  1055  CA  ILE A 157      25.372  39.081  25.720  1.00 49.85           C
ATOM  1056  CB  ILE A 157      26.185  39.009  27.030  1.00 50.01           C
ATOM  1057  CG2 ILE A 157      26.243  37.575  27.537  1.00 50.23           C
ATOM  1058  CG1 ILE A 157      27.589  39.570  26.801  1.00 50.25           C
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Figure 9T

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ATOM   1059  CD1 ILE A 157     28.382  38.852  25.727  1.00 50.65      C
ATOM   1060  C   ILE A 157     24.021  38.430  25.958  1.00 48.42      C
ATOM   1061  O   ILE A 157     23.185  38.955  26.689  1.00 48.14      O
ATOM   1062  N   GLU A 158     23.819  37.279  25.328  1.00 46.69      N
ATOM   1063  CA  GLU A 158     22.589  36.518  25.481  1.00 45.32      C
ATOM   1064  CB  GLU A 158     22.104  35.996  24.127  1.00 45.68      C
ATOM   1065  CG  GLU A 158     21.695  37.070  23.136  1.00 46.58      C
ATOM   1066  CD  GLU A 158     20.560  37.931  23.652  1.00 47.34      C
ATOM   1067  OE1 GLU A 158     19.576  37.369  24.179  1.00 47.28      O
ATOM   1068  OE2 GLU A 158     20.650  39.169  23.525  1.00 48.19      O
ATOM   1069  C   GLU A 158     22.920  35.336  26.385  1.00 43.98      C
ATOM   1070  O   GLU A 158     23.606  34.407  25.963  1.00 43.50      O
ATOM   1071  N   MET A 159     22.446  35.378  27.626  1.00 42.74      N
ATOM   1072  CA  MET A 159     22.711  34.295  28.570  1.00 41.56      C
ATOM   1073  CB  MET A 159     22.798  34.815  30.004  1.00 42.39      C
ATOM   1074  CG  MET A 159     24.088  35.514  30.371  1.00 44.11      C
ATOM   1075  SD  MET A 159     24.267  35.526  32.176  1.00 46.60      S
ATOM   1076  CE  MET A 159     22.851  36.541  32.649  1.00 46.03      C
ATOM   1077  C   MET A 159     21.648  33.218  28.532  1.00 40.26      C
ATOM   1078  O   MET A 159     20.464  33.501  28.365  1.00 39.98      O
ATOM   1079  N   LEU A 160     22.083  31.978  28.704  1.00 38.69      N
ATOM   1080  CA  LEU A 160     21.172  30.848  28.721  1.00 37.59      C
ATOM   1081  CB  LEU A 160     21.018  30.279  27.305  1.00 37.60      C
ATOM   1082  CG  LEU A 160     19.784  29.422  27.024  1.00 37.90      C
ATOM   1083  CD1 LEU A 160     19.650  29.202  25.519  1.00 37.83      C
ATOM   1084  CD2 LEU A 160     19.890  28.097  27.761  1.00 37.80      C
ATOM   1085  C   LEU A 160     21.750  29.800  29.677  1.00 36.65      C
ATOM   1086  O   LEU A 160     22.753  29.151  29.374  1.00 36.13      O
ATOM   1087  N   GLY A 161     21.125  29.663  30.844  1.00 35.74      N
ATOM   1088  CA  GLY A 161     21.586  28.699  31.831  1.00 34.53      C
ATOM   1089  C   GLY A 161     20.761  27.429  31.760  1.00 33.81      C
ATOM   1090  O   GLY A 161     19.531  27.483  31.773  1.00 33.71      O
ATOM   1091  N   SER A 162     21.424  26.281  31.688  1.00 32.70      N
ATOM   1092  CA  SER A 162     20.701  25.018  31.599  1.00 31.67      C
ATOM   1093  CB  SER A 162     20.570  24.587  30.134  1.00 30.98      C
ATOM   1094  OG  SER A 162     19.993  23.293  30.042  1.00 30.57      O
ATOM   1095  C   SER A 162     21.317  23.873  32.386  1.00 31.01      C
ATOM   1096  O   SER A 162     22.365  23.346  32.016  1.00 30.76      O
ATOM   1097  N   ALA A 163     20.650  23.477  33.464  1.00 30.33      N
ATOM   1098  CA  ALA A 163     21.125  22.369  34.273  1.00 29.58      C
ATOM   1099  CB  ALA A 163     20.385  22.341  35.603  1.00 30.07      C
ATOM   1100  C   ALA A 163     20.856  21.080  33.489  1.00 29.44      C
ATOM   1101  O   ALA A 163     21.569  20.089  33.631  1.00 28.92      O
ATOM   1102  N   GLU A 164     19.825  21.106  32.649  1.00 29.32      N
ATOM   1103  CA  GLU A 164     19.476  19.936  31.853  1.00 29.78      C
ATOM   1104  CB  GLU A 164     18.172  20.184  31.095  1.00 31.44      C
ATOM   1105  CG  GLU A 164     17.655  18.951  30.371  1.00 34.82      C
ATOM   1106  CD  GLU A 164     16.325  19.187  29.679  1.00 36.46      C
ATOM   1107  OE1 GLU A 164     15.678  20.222  29.958  1.00 38.07      O
ATOM   1108  OE2 GLU A 164     15.924  18.327  28.864  1.00 37.79      O
ATOM   1109  C   GLU A 164     20.582  19.575  30.859  1.00 29.30      C
ATOM   1110  O   GLU A 164     20.847  18.399  30.596  1.00 28.77      O
ATOM   1111  N   MET A 165     21.232  20.587  30.300  1.00 28.45      N
ATOM   1112  CA  MET A 165     22.298  20.317  29.345  1.00 28.20      C
ATOM   1113  CB  MET A 165     22.778  21.620  28.710  1.00 28.91      C
ATOM   1114  CG  MET A 165     23.570  21.398  27.431  1.00 30.59      C
ATOM   1115  SD  MET A 165     24.035  22.940  26.620  1.00 31.94      S
ATOM   1116  CE  MET A 165     22.494  23.418  25.882  1.00 31.97      C
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Figure 9U

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ATOM  1117  C   MET A 165     23.454  19.606  30.050  1.00 27.54      C
ATOM  1118  O   MET A 165     24.131  18.758  29.463  1.00 27.24      O
ATOM  1119  N   VAL A 166     23.678  19.952  31.314  1.00 26.73      N
ATOM  1120  CA  VAL A 166     24.740  19.311  32.073  1.00 26.74      C
ATOM  1121  CB  VAL A 166     24.841  19.883  33.500  1.00 26.61      C
ATOM  1122  CG1 VAL A 166     25.928  19.145  34.277  1.00 26.96      C
ATOM  1123  CG2 VAL A 166     25.149  21.373  33.441  1.00 26.49      C
ATOM  1124  C   VAL A 166     24.424  17.820  32.152  1.00 27.07      C
ATOM  1125  O   VAL A 166     25.301  16.980  31.972  1.00 26.02      O
ATOM  1126  N   GLU A 167     23.158  17.506  32.417  1.00 27.89      N
ATOM  1127  CA  GLU A 167     22.714  16.121  32.517  1.00 29.12      C
ATOM  1128  CB  GLU A 167     21.260  16.062  33.002  1.00 31.04      C
ATOM  1129  CG  GLU A 167     21.099  16.378  34.471  1.00 34.37      C
ATOM  1130  CD  GLU A 167     22.033  15.552  35.344  1.00 36.89      C
ATOM  1131  OE1 GLU A 167     22.130  14.321  35.130  1.00 38.46      O
ATOM  1132  OE2 GLU A 167     22.675  16.130  36.249  1.00 38.74      O
ATOM  1133  C   GLU A 167     22.842  15.390  31.189  1.00 28.28      C
ATOM  1134  O   GLU A 167     23.150  14.200  31.153  1.00 28.26      O
ATOM  1135  N   LEU A 168     22.598  16.100  30.095  1.00 28.21      N
ATOM  1136  CA  LEU A 168     22.712  15.494  28.779  1.00 28.05      C
ATOM  1137  CB  LEU A 168     22.265  16.487  27.697  1.00 28.07      C
ATOM  1138  CG  LEU A 168     20.756  16.747  27.683  1.00 28.26      C
ATOM  1139  CD1 LEU A 168     20.422  17.814  26.662  1.00 28.45      C
ATOM  1140  CD2 LEU A 168     20.025  15.452  27.366  1.00 28.49      C
ATOM  1141  C   LEU A 168     24.163  15.077  28.568  1.00 27.93      C
ATOM  1142  O   LEU A 168     24.438  13.999  28.037  1.00 28.11      O
ATOM  1143  N   ALA A 169     25.089  15.926  29.007  1.00 27.73      N
ATOM  1144  CA  ALA A 169     26.515  15.632  28.873  1.00 28.12      C
ATOM  1145  CB  ALA A 169     27.358  16.852  29.288  1.00 27.69      C
ATOM  1146  C   ALA A 169     26.859  14.426  29.746  1.00 28.18      C
ATOM  1147  O   ALA A 169     27.572  13.519  29.311  1.00 28.29      O
ATOM  1148  N   GLU A 170     26.357  14.415  30.978  1.00 28.76      N
ATOM  1149  CA  GLU A 170     26.610  13.285  31.873  1.00 29.18      C
ATOM  1150  CB  GLU A 170     25.898  13.480  33.218  1.00 29.14      C
ATOM  1151  CG  GLU A 170     26.581  14.460  34.167  1.00 29.02      C
ATOM  1152  CD  GLU A 170     27.862  13.903  34.788  1.00 29.97      C
ATOM  1153  OE1 GLU A 170     28.793  14.700  35.045  1.00 29.30      O
ATOM  1154  OE2 GLU A 170     27.939  12.676  35.032  1.00 30.01      O
ATOM  1155  C   GLU A 170     26.099  12.011  31.205  1.00 29.51      C
ATOM  1156  O   GLU A 170     26.824  11.025  31.090  1.00 29.71      O
ATOM  1157  N   ALA A 171     24.848  12.042  30.752  1.00 29.94      N
ATOM  1158  CA  ALA A 171     24.253  10.883  30.094  1.00 30.26      C
ATOM  1159  CB  ALA A 171     22.868  11.234  29.572  1.00 30.29      C
ATOM  1160  C   ALA A 171     25.124  10.394  28.947  1.00 30.81      C
ATOM  1161  O   ALA A 171     25.412   9.201  28.834  1.00 31.13      O
ATOM  1162  N   LYS A 172     25.546  11.316  28.091  1.00 31.06      N
ATOM  1163  CA  LYS A 172     26.366  10.947  26.950  1.00 32.12      C
ATOM  1164  CB  LYS A 172     26.795  12.192  26.171  1.00 32.06      C
ATOM  1165  CG  LYS A 172     27.626  11.871  24.940  1.00 32.46      C
ATOM  1166  CD  LYS A 172     28.013  13.136  24.180  1.00 32.50      C
ATOM  1167  CE  LYS A 172     28.815  12.800  22.932  1.00 33.01      C
ATOM  1168  NZ  LYS A 172     29.159  14.022  22.167  1.00 32.96      N
ATOM  1169  C   LYS A 172     27.597  10.131  27.326  1.00 32.64      C
ATOM  1170  O   LYS A 172     27.829   9.062  26.757  1.00 32.92      O
ATOM  1171  N   LEU A 173     28.387  10.620  28.276  1.00 33.14      N
ATOM  1172  CA  LEU A 173     29.587   9.897  28.669  1.00 34.31      C
ATOM  1173  CB  LEU A 173     30.552  10.812  29.433  1.00 34.17      C
ATOM  1174  CG  LEU A 173     31.093  12.078  28.747  1.00 34.37      C
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Figure 9V

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ATOM  1175 CD1 LEU A 173    32.576  12.212  29.062  1.00 33.96      C
ATOM  1176 CD2 LEU A 173    30.880  12.025  27.247  1.00 34.33      C
ATOM  1177 C   LEU A 173    29.278   8.653  29.496  1.00 35.30      C
ATOM  1178 O   LEU A 173    30.172   7.870  29.805  1.00 35.42      O
ATOM  1179 N   HIS A 174    28.015   8.473  29.864  1.00 36.72      N
ATOM  1180 CA  HIS A 174    27.630   7.293  30.626  1.00 38.16      C
ATOM  1181 CB  HIS A 174    26.560   7.644  31.664  1.00 37.76      C
ATOM  1182 CG  HIS A 174    27.124   8.213  32.929  1.00 37.39      C
ATOM  1183 CD2 HIS A 174    27.348   9.494  33.308  1.00 37.15      C
ATOM  1184 ND1 HIS A 174    27.602   7.422  33.953  1.00 37.82      N
ATOM  1185 CE1 HIS A 174    28.095   8.192  34.907  1.00 37.44      C
ATOM  1186 NE2 HIS A 174    27.955   9.453  34.540  1.00 37.12      N
ATOM  1187 C   HIS A 174    27.130   6.219  29.669  1.00 39.31      C
ATOM  1188 O   HIS A 174    26.810   5.108  30.083  1.00 39.72      O
ATOM  1189 N   GLY A 175    27.073   6.560  28.384  1.00 40.42      N
ATOM  1190 CA  GLY A 175    26.639   5.597  27.387  1.00 41.81      C
ATOM  1191 C   GLY A 175    25.287   5.845  26.747  1.00 43.00      C
ATOM  1192 O   GLY A 175    24.886   5.105  25.846  1.00 43.03      O
ATOM  1193 N   GLU A 176    24.571   6.868  27.204  1.00 43.77      N
ATOM  1194 CA  GLU A 176    23.266   7.173  26.629  1.00 45.02      C
ATOM  1195 CB  GLU A 176    22.324   7.762  27.686  1.00 46.03      C
ATOM  1196 CG  GLU A 176    21.921   6.795  28.792  1.00 47.96      C
ATOM  1197 CD  GLU A 176    22.955   6.689  29.898  1.00 49.25      C
ATOM  1198 OE1 GLU A 176    23.169   7.694  30.614  1.00 49.83      O
ATOM  1199 OE2 GLU A 176    23.552   5.601  30.055  1.00 50.12      O
ATOM  1200 C   GLU A 176    23.413   8.153  25.474  1.00 45.17      C
ATOM  1201 O   GLU A 176    24.327   8.975  25.459  1.00 45.70      O
ATOM  1202 N   ASP A 177    22.512   8.059  24.503  1.00 45.24      N
ATOM  1203 CA  ASP A 177    22.545   8.938  23.342  1.00 44.89      C
ATOM  1204 CB  ASP A 177    21.869   8.253  22.157  1.00 46.19      C
ATOM  1205 CG  ASP A 177    22.460   6.882  21.871  1.00 47.31      C
ATOM  1206 OD1 ASP A 177    23.559   6.818  21.272  1.00 47.70      O
ATOM  1207 OD2 ASP A 177    21.831   5.873  22.267  1.00 48.01      O
ATOM  1208 C   ASP A 177    21.833  10.238  23.672  1.00 43.98      C
ATOM  1209 O   ASP A 177    20.814  10.243  24.357  1.00 44.07      O
ATOM  1210 N   VAL A 178    22.381  11.342  23.186  1.00 42.87      N
ATOM  1211 CA  VAL A 178    21.800  12.649  23.441  1.00 41.57      C
ATOM  1212 CB  VAL A 178    22.852  13.765  23.229  1.00 41.43      C
ATOM  1213 CG1 VAL A 178    22.253  15.120  23.567  1.00 40.77      C
ATOM  1214 CG2 VAL A 178    24.085  13.484  24.083  1.00 41.33      C
ATOM  1215 C   VAL A 178    20.608  12.913  22.524  1.00 40.74      C
ATOM  1216 O   VAL A 178    20.715  12.801  21.305  1.00 40.65      O
ATOM  1217 N   SER A 179    19.471  13.260  23.118  1.00 40.12      N
ATOM  1218 CA  SER A 179    18.271  13.564  22.346  1.00 39.22      C
ATOM  1219 CB  SER A 179    17.032  13.517  23.234  1.00 39.19      C
ATOM  1220 OG  SER A 179    15.955  14.187  22.604  1.00 39.12      O
ATOM  1221 C   SER A 179    18.397  14.957  21.751  1.00 38.78      C
ATOM  1222 O   SER A 179    18.419  15.950  22.482  1.00 38.57      O
ATOM  1223 N   LEU A 180    18.480  15.036  20.427  1.00 38.11      N
ATOM  1224 CA  LEU A 180    18.602  16.330  19.772  1.00 37.12      C
ATOM  1225 CB  LEU A 180    18.859  16.153  18.276  1.00 37.25      C
ATOM  1226 CG  LEU A 180    20.159  15.430  17.903  1.00 37.36      C
ATOM  1227 CD1 LEU A 180    20.354  15.483  16.394  1.00 37.56      C
ATOM  1228 CD2 LEU A 180    21.344  16.082  18.615  1.00 37.57      C
ATOM  1229 C   LEU A 180    17.355  17.173  19.995  1.00 36.72      C
ATOM  1230 O   LEU A 180    17.433  18.398  20.045  1.00 36.33      O
ATOM  1231 N   ASP A 181    16.203  16.523  20.136  1.00 36.44      N
ATOM  1232 CA  ASP A 181    14.966  17.256  20.366  1.00 36.07      C
```

Figure 9W

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ATOM  1233  CB  ASP A 181     13.754  16.319  20.311  1.00 37.55      C
ATOM  1234  CG  ASP A 181     13.486  15.790  18.909  1.00 38.95      C
ATOM  1235  OD1 ASP A 181     13.589  16.570  17.937  1.00 39.74      O
ATOM  1236  OD2 ASP A 181     13.158  14.594  18.777  1.00 40.38      O
ATOM  1237  C   ASP A 181     15.014  17.971  21.714  1.00 34.99      C
ATOM  1238  O   ASP A 181     14.491  19.074  21.859  1.00 34.62      O
ATOM  1239  N   ALA A 182     15.638  17.337  22.702  1.00 34.20      N
ATOM  1240  CA  ALA A 182     15.766  17.939  24.026  1.00 33.44      C
ATOM  1241  CB  ALA A 182     16.388  16.937  25.003  1.00 33.26      C
ATOM  1242  C   ALA A 182     16.645  19.186  23.910  1.00 32.88      C
ATOM  1243  O   ALA A 182     16.362  20.216  24.514  1.00 32.37      O
ATOM  1244  N   LEU A 183     17.714  19.085  23.124  1.00 32.52      N
ATOM  1245  CA  LEU A 183     18.614  20.214  22.915  1.00 31.97      C
ATOM  1246  CB  LEU A 183     19.823  19.796  22.080  1.00 32.53      C
ATOM  1247  CG  LEU A 183     21.089  19.365  22.816  1.00 33.44      C
ATOM  1248  CD1 LEU A 183     22.184  19.088  21.785  1.00 33.67      C
ATOM  1249  CD2 LEU A 183     21.533  20.463  23.787  1.00 33.50      C
ATOM  1250  C   LEU A 183     17.913  21.366  22.213  1.00 31.47      C
ATOM  1251  O   LEU A 183     18.060  22.524  22.609  1.00 31.07      O
ATOM  1252  N   LYS A 184     17.160  21.050  21.163  1.00 30.86      N
ATOM  1253  CA  LYS A 184     16.443  22.075  20.413  1.00 31.16      C
ATOM  1254  CB  LYS A 184     15.651  21.445  19.262  1.00 31.63      C
ATOM  1255  CG  LYS A 184     16.513  20.868  18.158  1.00 32.93      C
ATOM  1256  CD  LYS A 184     15.675  20.111  17.139  1.00 33.75      C
ATOM  1257  CE  LYS A 184     16.556  19.416  16.115  1.00 34.92      C
ATOM  1258  NZ  LYS A 184     15.750  18.568  15.178  1.00 35.78      N
ATOM  1259  C   LYS A 184     15.487  22.824  21.328  1.00 30.89      C
ATOM  1260  O   LYS A 184     15.307  24.033  21.199  1.00 30.37      O
ATOM  1261  N   ARG A 185     14.869  22.090  22.244  1.00 30.97      N
ATOM  1262  CA  ARG A 185     13.926  22.680  23.183  1.00 31.66      C
ATOM  1263  CB  ARG A 185     13.260  21.576  24.011  1.00 32.95      C
ATOM  1264  CG  ARG A 185     12.273  22.095  25.045  1.00 35.19      C
ATOM  1265  CD  ARG A 185     11.071  22.763  24.385  1.00 36.95      C
ATOM  1266  NE  ARG A 185     10.276  23.497  25.366  1.00 38.48      N
ATOM  1267  CZ  ARG A 185     10.678  24.616  25.959  1.00 39.27      C
ATOM  1268  NH1 ARG A 185     11.864  25.138  25.668  1.00 39.25      N
ATOM  1269  NH2 ARG A 185      9.901  25.206  26.857  1.00 40.18      N
ATOM  1270  C   ARG A 185     14.667  23.645  24.101  1.00 30.92      C
ATOM  1271  O   ARG A 185     14.239  24.781  24.313  1.00 30.74      O
ATOM  1272  N   ILE A 186     15.789  23.186  24.642  1.00 30.14      N
ATOM  1273  CA  ILE A 186     16.585  24.022  25.528  1.00 29.32      C
ATOM  1274  CB  ILE A 186     17.832  23.252  26.037  1.00 29.04      C
ATOM  1275  CG2 ILE A 186     18.741  24.190  26.829  1.00 29.20      C
ATOM  1276  CG1 ILE A 186     17.389  22.058  26.894  1.00 29.51      C
ATOM  1277  CD1 ILE A 186     18.534  21.148  27.330  1.00 29.37      C
ATOM  1278  C   ILE A 186     17.037  25.285  24.792  1.00 28.71      C
ATOM  1279  O   ILE A 186     17.015  26.380  25.351  1.00 28.31      O
ATOM  1280  N   LEU A 187     17.435  25.130  23.532  1.00 28.36      N
ATOM  1281  CA  LEU A 187     17.911  26.257  22.733  1.00 28.42      C
ATOM  1282  CB  LEU A 187     18.998  25.772  21.757  1.00 28.23      C
ATOM  1283  CG  LEU A 187     20.268  25.207  22.409  1.00 28.51      C
ATOM  1284  CD1 LEU A 187     21.125  24.483  21.376  1.00 28.72      C
ATOM  1285  CD2 LEU A 187     21.049  26.337  23.051  1.00 28.48      C
ATOM  1286  C   LEU A 187     16.814  26.996  21.956  1.00 28.77      C
ATOM  1287  O   LEU A 187     17.105  27.913  21.189  1.00 27.81      O
ATOM  1288  N   ARG A 188     15.559  26.611  22.173  1.00 29.44      N
ATOM  1289  CA  ARG A 188     14.437  27.232  21.470  1.00 30.59      C
ATOM  1290  CB  ARG A 188     13.096  26.759  22.066  1.00 31.00      C
```

Figure 9X

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ATOM  1291  CG  ARG A 188      11.880  27.044  21.161  1.00 31.92      C
ATOM  1292  CD  ARG A 188      10.591  26.415  21.694  1.00 32.72      C
ATOM  1293  NE  ARG A 188      10.065  27.111  22.869  1.00 33.40      N
ATOM  1294  CZ  ARG A 188       8.896  26.834  23.440  1.00 33.80      C
ATOM  1295  NH1 ARG A 188       8.127  25.871  22.951  1.00 34.90      N
ATOM  1296  NH2 ARG A 188       8.486  27.525  24.492  1.00 34.07      N
ATOM  1297  C   ARG A 188      14.522  28.761  21.479  1.00 31.15      C
ATOM  1298  O   ARG A 188      14.384  29.394  20.437  1.00 31.37      O
ATOM  1299  N   PRO A 189      14.778  29.373  22.652  1.00 31.69      N
ATOM  1300  CD  PRO A 189      15.085  28.750  23.953  1.00 31.58      C
ATOM  1301  CA  PRO A 189      14.877  30.835  22.741  1.00 32.00      C
ATOM  1302  CB  PRO A 189      15.460  31.055  24.134  1.00 32.34      C
ATOM  1303  CG  PRO A 189      14.931  29.907  24.908  1.00 32.12      C
ATOM  1304  C   PRO A 189      15.781  31.423  21.661  1.00 32.69      C
ATOM  1305  O   PRO A 189      15.444  32.428  21.024  1.00 33.41      O
ATOM  1306  N   TRP A 190      16.937  30.795  21.467  1.00 32.33      N
ATOM  1307  CA  TRP A 190      17.902  31.251  20.478  1.00 32.66      C
ATOM  1308  CB  TRP A 190      19.276  30.637  20.767  1.00 31.96      C
ATOM  1309  CG  TRP A 190      19.946  31.238  21.972  1.00 31.74      C
ATOM  1310  CD2 TRP A 190      21.261  30.942  22.461  1.00 31.19      C
ATOM  1311  CE2 TRP A 190      21.475  31.752  23.597  1.00 31.14      C
ATOM  1312  CE3 TRP A 190      22.278  30.070  22.048  1.00 31.17      C
ATOM  1313  CD1 TRP A 190      19.432  32.187  22.808  1.00 31.47      C
ATOM  1314  NE1 TRP A 190      20.343  32.502  23.786  1.00 31.75      N
ATOM  1315  CZ2 TRP A 190      22.666  31.719  24.327  1.00 30.64      C
ATOM  1316  CZ3 TRP A 190      23.468  30.038  22.777  1.00 30.63      C
ATOM  1317  CH2 TRP A 190      23.647  30.858  23.903  1.00 30.76      C
ATOM  1318  C   TRP A 190      17.473  30.936  19.053  1.00 32.80      C
ATOM  1319  O   TRP A 190      17.678  31.739  18.151  1.00 33.14      O
ATOM  1320  N   LEU A 191      16.875  29.769  18.853  1.00 33.23      N
ATOM  1321  CA  LEU A 191      16.420  29.384  17.525  1.00 34.12      C
ATOM  1322  CB  LEU A 191      15.997  27.913  17.514  1.00 34.10      C
ATOM  1323  CG  LEU A 191      17.133  26.920  17.767  1.00 34.63      C
ATOM  1324  CD1 LEU A 191      16.571  25.512  17.926  1.00 34.77      C
ATOM  1325  CD2 LEU A 191      18.124  26.985  16.605  1.00 34.84      C
ATOM  1326  C   LEU A 191      15.264  30.262  17.047  1.00 34.32      C
ATOM  1327  O   LEU A 191      14.943  30.270  15.864  1.00 34.60      O
ATOM  1328  N   ARG A 192      14.640  31.000  17.962  1.00 34.66      N
ATOM  1329  CA  ARG A 192      13.532  31.879  17.584  1.00 35.36      C
ATOM  1330  CB  ARG A 192      12.417  31.827  18.630  1.00 35.21      C
ATOM  1331  CG  ARG A 192      11.568  30.569  18.575  1.00 34.86      C
ATOM  1332  CD  ARG A 192      10.556  30.560  19.709  1.00 34.91      C
ATOM  1333  NE  ARG A 192       9.624  29.440  19.608  1.00 35.35      N
ATOM  1334  CZ  ARG A 192       8.670  29.181  20.500  1.00 34.80      C
ATOM  1335  NH1 ARG A 192       8.528  29.960  21.563  1.00 34.29      N
ATOM  1336  NH2 ARG A 192       7.851  28.152  20.318  1.00 34.13      N
ATOM  1337  C   ARG A 192      13.966  33.328  17.393  1.00 35.93      C
ATOM  1338  O   ARG A 192      13.130  34.204  17.168  1.00 36.00      O
ATOM  1339  N   MET A 193      15.270  33.579  17.479  1.00 36.28      N
ATOM  1340  CA  MET A 193      15.797  34.930  17.316  1.00 36.54      C
ATOM  1341  CB  MET A 193      17.139  35.070  18.045  1.00 36.79      C
ATOM  1342  CG  MET A 193      17.038  35.165  19.564  1.00 36.88      C
ATOM  1343  SD  MET A 193      18.669  35.278  20.352  1.00 37.53      S
ATOM  1344  CE  MET A 193      19.079  37.031  20.122  1.00 36.86      C
ATOM  1345  C   MET A 193      15.987  35.306  15.848  1.00 36.67      C
ATOM  1346  O   MET A 193      16.368  34.467  15.025  1.00 36.46      O
ATOM  1347  N   LYS A 194      15.715  36.570  15.526  1.00 37.01      N
ATOM  1348  CA  LYS A 194      15.889  37.067  14.163  1.00 37.69      C
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Figure 9Y

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ATOM  1349  CB  LYS A 194      15.478  38.545  14.064  1.00 38.05           C
ATOM  1350  CG  LYS A 194      15.613  39.121  12.654  1.00 38.80           C
ATOM  1351  CD  LYS A 194      16.261  40.515  12.623  1.00 39.92           C
ATOM  1352  CE  LYS A 194      15.284  41.663  12.887  1.00 40.54           C
ATOM  1353  NZ  LYS A 194      14.817  41.801  14.299  1.00 41.22           N
ATOM  1354  C   LYS A 194      17.374  36.928  13.832  1.00 37.73           C
ATOM  1355  O   LYS A 194      17.757  36.399  12.787  1.00 37.39           O
ATOM  1356  N   GLU A 195      18.206  37.413  14.744  1.00 38.33           N
ATOM  1357  CA  GLU A 195      19.650  37.332  14.574  1.00 38.43           C
ATOM  1358  CB  GLU A 195      20.248  38.722  14.361  1.00 39.41           C
ATOM  1359  CG  GLU A 195      21.766  38.698  14.281  1.00 41.23           C
ATOM  1360  CD  GLU A 195      22.348  39.961  13.690  1.00 42.54           C
ATOM  1361  OE1 GLU A 195      21.953  41.066  14.125  1.00 43.29           O
ATOM  1362  OE2 GLU A 195      23.211  39.844  12.792  1.00 43.45           O
ATOM  1363  C   GLU A 195      20.268  36.688  15.810  1.00 37.55           C
ATOM  1364  O   GLU A 195      20.596  37.368  16.781  1.00 37.40           O
ATOM  1365  N   PRO A 196      20.422  35.358  15.792  1.00 36.88           N
ATOM  1366  CD  PRO A 196      20.121  34.417  14.697  1.00 37.02           C
ATOM  1367  CA  PRO A 196      21.006  34.659  16.940  1.00 36.26           C
ATOM  1368  CB  PRO A 196      20.744  33.191  16.611  1.00 36.49           C
ATOM  1369  CG  PRO A 196      20.877  33.165  15.122  1.00 37.04           C
ATOM  1370  C   PRO A 196      22.491  34.973  17.078  1.00 35.39           C
ATOM  1371  O   PRO A 196      23.105  35.530  16.166  1.00 35.42           O
ATOM  1372  N   PRO A 197      23.089  34.626  18.228  1.00 34.89           N
ATOM  1373  CD  PRO A 197      22.518  33.900  19.374  1.00 34.65           C
ATOM  1374  CA  PRO A 197      24.517  34.894  18.438  1.00 34.16           C
ATOM  1375  CB  PRO A 197      24.789  34.288  19.820  1.00 34.06           C
ATOM  1376  CG  PRO A 197      23.457  34.284  20.480  1.00 34.48           C
ATOM  1377  C   PRO A 197      25.334  34.192  17.366  1.00 33.22           C
ATOM  1378  O   PRO A 197      25.018  33.067  16.991  1.00 33.54           O
ATOM  1379  N   ASP A 198      26.376  34.838  16.857  1.00 32.64           N
ATOM  1380  CA  ASP A 198      27.200  34.173  15.861  1.00 32.00           C
ATOM  1381  CB  ASP A 198      27.669  35.169  14.782  1.00 32.92           C
ATOM  1382  CG  ASP A 198      28.741  36.136  15.269  1.00 34.20           C
ATOM  1383  OD1 ASP A 198      28.889  36.334  16.497  1.00 34.32           O
ATOM  1384  OD2 ASP A 198      29.433  36.718  14.394  1.00 34.48           O
ATOM  1385  C   ASP A 198      28.379  33.517  16.590  1.00 30.70           C
ATOM  1386  O   ASP A 198      29.151  32.754  16.008  1.00 30.48           O
ATOM  1387  N   THR A 199      28.477  33.797  17.885  1.00 29.73           N
ATOM  1388  CA  THR A 199      29.541  33.245  18.728  1.00 28.32           C
ATOM  1389  CB  THR A 199      30.609  34.317  19.009  1.00 28.44           C
ATOM  1390  OG1 THR A 199      31.040  34.892  17.767  1.00 28.45           O
ATOM  1391  CG2 THR A 199      31.817  33.703  19.712  1.00 27.68           C
ATOM  1392  C   THR A 199      28.925  32.774  20.050  1.00 27.54           C
ATOM  1393  O   THR A 199      28.258  33.544  20.731  1.00 27.62           O
ATOM  1394  N   VAL A 200      29.137  31.509  20.408  1.00 26.67           N
ATOM  1395  CA  VAL A 200      28.573  30.975  21.645  1.00 25.45           C
ATOM  1396  CB  VAL A 200      27.603  29.794  21.368  1.00 25.29           C
ATOM  1397  CG1 VAL A 200      27.103  29.205  22.688  1.00 24.41           C
ATOM  1398  CG2 VAL A 200      26.410  30.273  20.533  1.00 25.16           C
ATOM  1399  C   VAL A 200      29.665  30.485  22.586  1.00 24.96           C
ATOM  1400  O   VAL A 200      30.457  29.615  22.228  1.00 25.00           O
ATOM  1401  N   VAL A 201      29.692  31.050  23.787  1.00 24.00           N
ATOM  1402  CA  VAL A 201      30.672  30.680  24.803  1.00 24.07           C
ATOM  1403  CB  VAL A 201      30.931  31.850  25.784  1.00 23.91           C
ATOM  1404  CG1 VAL A 201      31.872  31.401  26.907  1.00 23.25           C
ATOM  1405  CG2 VAL A 201      31.527  33.032  25.035  1.00 23.70           C
ATOM  1406  C   VAL A 201      30.151  29.506  25.620  1.00 23.96           C
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Figure 9Z

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ATOM  1407  O   VAL A 201     29.044  29.551  26.144  1.00 24.03      O
ATOM  1408  N   LEU A 202     30.937  28.445  25.711  1.00 24.28      N
ATOM  1409  CA  LEU A 202     30.531  27.304  26.519  1.00 24.52      C
ATOM  1410  CB  LEU A 202     31.091  26.010  25.927  1.00 24.85      C
ATOM  1411  CG  LEU A 202     30.634  25.793  24.479  1.00 24.66      C
ATOM  1412  CD1 LEU A 202     31.126  24.450  23.954  1.00 25.52      C
ATOM  1413  CD2 LEU A 202     29.115  25.869  24.418  1.00 24.68      C
ATOM  1414  C   LEU A 202     31.123  27.596  27.890  1.00 24.97      C
ATOM  1415  O   LEU A 202     32.318  27.377  28.124  1.00 25.27      O
ATOM  1416  N   GLY A 203     30.283  28.132  28.772  1.00 25.47      N
ATOM  1417  CA  GLY A 203     30.708  28.498  30.114  1.00 26.68      C
ATOM  1418  C   GLY A 203     30.468  27.425  31.157  1.00 27.26      C
ATOM  1419  O   GLY A 203     30.282  27.711  32.337  1.00 28.58      O
ATOM  1420  N   CYS A 204     30.441  26.182  30.704  1.00 27.73      N
ATOM  1421  CA  CYS A 204     30.273  25.034  31.582  1.00 27.40      C
ATOM  1422  CB  CYS A 204     28.824  24.551  31.568  1.00 28.28      C
ATOM  1423  SG  CYS A 204     28.483  23.277  32.788  1.00 29.75      S
ATOM  1424  C   CYS A 204     31.200  23.998  30.959  1.00 26.65      C
ATOM  1425  O   CYS A 204     31.088  23.705  29.768  1.00 26.53      O
ATOM  1426  N   THR A 205     32.130  23.455  31.740  1.00 25.96      N
ATOM  1427  CA  THR A 205     33.072  22.481  31.188  1.00 25.54      C
ATOM  1428  CB  THR A 205     34.179  22.112  32.213  1.00 25.97      C
ATOM  1429  OG1 THR A 205     33.604  21.417  33.326  1.00 25.47      O
ATOM  1430  CG2 THR A 205     34.866  23.376  32.720  1.00 26.26      C
ATOM  1431  C   THR A 205     32.398  21.209  30.671  1.00 25.02      C
ATOM  1432  O   THR A 205     33.020  20.402  29.978  1.00 25.08      O
ATOM  1433  N   HIS A 206     31.126  21.024  31.004  1.00 25.00      N
ATOM  1434  CA  HIS A 206     30.389  19.861  30.507  1.00 25.50      C
ATOM  1435  CB  HIS A 206     29.096  19.644  31.301  1.00 25.48      C
ATOM  1436  CG  HIS A 206     29.243  18.752  32.496  1.00 25.77      C
ATOM  1437  CD2 HIS A 206     28.818  17.485  32.715  1.00 26.12      C
ATOM  1438  ND1 HIS A 206     29.853  19.158  33.664  1.00 26.12      N
ATOM  1439  CE1 HIS A 206     29.794  18.182  34.552  1.00 26.27      C
ATOM  1440  NE2 HIS A 206     29.171  17.156  34.001  1.00 25.97      N
ATOM  1441  C   HIS A 206     29.990  20.056  29.038  1.00 25.23      C
ATOM  1442  O   HIS A 206     29.915  19.096  28.261  1.00 24.85      O
ATOM  1443  N   PHE A 207     29.739  21.305  28.661  1.00 25.12      N
ATOM  1444  CA  PHE A 207     29.259  21.602  27.314  1.00 24.78      C
ATOM  1445  CB  PHE A 207     28.765  23.059  27.262  1.00 24.50      C
ATOM  1446  CG  PHE A 207     27.625  23.346  28.223  1.00 24.94      C
ATOM  1447  CD1 PHE A 207     27.171  24.651  28.422  1.00 24.92      C
ATOM  1448  CD2 PHE A 207     27.019  22.311  28.945  1.00 25.02      C
ATOM  1449  CE1 PHE A 207     26.137  24.924  29.322  1.00 24.91      C
ATOM  1450  CE2 PHE A 207     25.984  22.574  29.848  1.00 24.68      C
ATOM  1451  CZ  PHE A 207     25.544  23.881  30.037  1.00 24.50      C
ATOM  1452  C   PHE A 207     30.139  21.263  26.117  1.00 24.23      C
ATOM  1453  O   PHE A 207     29.624  20.794  25.105  1.00 24.49      O
ATOM  1454  N   PRO A 208     31.467  21.485  26.199  1.00 24.05      N
ATOM  1455  CD  PRO A 208     32.268  22.196  27.216  1.00 23.52      C
ATOM  1456  CA  PRO A 208     32.292  21.140  25.035  1.00 23.79      C
ATOM  1457  CB  PRO A 208     33.709  21.443  25.519  1.00 23.37      C
ATOM  1458  CG  PRO A 208     33.497  22.617  26.415  1.00 23.62      C
ATOM  1459  C   PRO A 208     32.111  19.665  24.650  1.00 23.75      C
ATOM  1460  O   PRO A 208     32.307  19.283  23.496  1.00 23.71      O
ATOM  1461  N   LEU A 209     31.731  18.846  25.628  1.00 24.35      N
ATOM  1462  CA  LEU A 209     31.510  17.416  25.400  1.00 24.73      C
ATOM  1463  CB  LEU A 209     31.225  16.703  26.730  1.00 24.44      C
ATOM  1464  CG  LEU A 209     32.351  16.705  27.763  1.00 24.17      C
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Figure 9AA

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ATOM  1465 CD1 LEU A 209    31.856 16.084 29.055 1.00 24.39      C
ATOM  1466 CD2 LEU A 209    33.546 15.940 27.213 1.00 25.04      C
ATOM  1467 C   LEU A 209    30.330 17.193 24.453 1.00 24.96      C
ATOM  1468 O   LEU A 209    30.185 16.115 23.871 1.00 25.40      O
ATOM  1469 N   LEU A 210    29.492 18.214 24.311 1.00 25.40      N
ATOM  1470 CA  LEU A 210    28.313 18.150 23.445 1.00 26.09      C
ATOM  1471 CB  LEU A 210    27.091 18.700 24.187 1.00 26.08      C
ATOM  1472 CG  LEU A 210    26.612 17.931 25.424 1.00 26.43      C
ATOM  1473 CD1 LEU A 210    25.590 18.754 26.165 1.00 26.49      C
ATOM  1474 CD2 LEU A 210    26.031 16.587 25.006 1.00 26.75      C
ATOM  1475 C   LEU A 210    28.513 18.956 22.165 1.00 26.97      C
ATOM  1476 O   LEU A 210    27.551 19.238 21.443 1.00 26.49      O
ATOM  1477 N   GLN A 211    29.754 19.325 21.877 1.00 27.84      N
ATOM  1478 CA  GLN A 211    30.018 20.125 20.689 1.00 29.76      C
ATOM  1479 CB  GLN A 211    31.525 20.241 20.426 1.00 31.43      C
ATOM  1480 CG  GLN A 211    31.822 21.058 19.169 1.00 35.04      C
ATOM  1481 CD  GLN A 211    33.278 21.444 19.027 1.00 36.79      C
ATOM  1482 OE1 GLN A 211    33.814 22.205 19.840 1.00 38.21      O
ATOM  1483 NE2 GLN A 211    33.929 20.926 17.985 1.00 37.92      N
ATOM  1484 C   GLN A 211    29.319 19.624 19.428 1.00 29.78      C
ATOM  1485 O   GLN A 211    28.629 20.390 18.757 1.00 29.75      O
ATOM  1486 N   GLU A 212    29.482 18.346 19.104 1.00 30.23      N
ATOM  1487 CA  GLU A 212    28.857 17.805 17.898 1.00 31.41      C
ATOM  1488 CB  GLU A 212    29.173 16.312 17.750 1.00 33.48      C
ATOM  1489 CG  GLU A 212    28.789 15.739 16.391 1.00 36.83      C
ATOM  1490 CD  GLU A 212    29.709 14.609 15.940 1.00 38.98      C
ATOM  1491 OE1 GLU A 212    30.921 14.860 15.738 1.00 40.36      O
ATOM  1492 OE2 GLU A 212    29.223 13.468 15.786 1.00 40.67      O
ATOM  1493 C   GLU A 212    27.348 18.023 17.894 1.00 30.99      C
ATOM  1494 O   GLU A 212    26.791 18.548 16.928 1.00 30.68      O
ATOM  1495 N   GLU A 213    26.692 17.628 18.983 1.00 30.23      N
ATOM  1496 CA  GLU A 213    25.253 17.788 19.103 1.00 29.95      C
ATOM  1497 CB  GLU A 213    24.760 17.214 20.436 1.00 30.26      C
ATOM  1498 CG  GLU A 213    24.844 15.697 20.570 1.00 31.58      C
ATOM  1499 CD  GLU A 213    26.237 15.179 20.909 1.00 32.64      C
ATOM  1500 OE1 GLU A 213    27.150 15.992 21.177 1.00 32.86      O
ATOM  1501 OE2 GLU A 213    26.412 13.942 20.915 1.00 33.12      O
ATOM  1502 C   GLU A 213    24.840 19.258 19.005 1.00 29.41      C
ATOM  1503 O   GLU A 213    23.857 19.587 18.338 1.00 29.01      O
ATOM  1504 N   LEU A 214    25.580 20.137 19.681 1.00 28.84      N
ATOM  1505 CA  LEU A 214    25.268 21.567 19.656 1.00 28.43      C
ATOM  1506 CB  LEU A 214    26.216 22.348 20.570 1.00 28.13      C
ATOM  1507 CG  LEU A 214    25.977 22.173 22.075 1.00 27.63      C
ATOM  1508 CD1 LEU A 214    27.109 22.818 22.862 1.00 27.49      C
ATOM  1509 CD2 LEU A 214    24.626 22.791 22.447 1.00 27.85      C
ATOM  1510 C   LEU A 214    25.348 22.136 18.247 1.00 28.83      C
ATOM  1511 O   LEU A 214    24.507 22.937 17.845 1.00 27.87      O
ATOM  1512 N   LEU A 215    26.356 21.713 17.498 1.00 29.30      N
ATOM  1513 CA  LEU A 215    26.528 22.202 16.142 1.00 30.96      C
ATOM  1514 CB  LEU A 215    27.918 21.822 15.630 1.00 30.54      C
ATOM  1515 CG  LEU A 215    29.025 22.593 16.358 1.00 30.81      C
ATOM  1516 CD1 LEU A 215    30.386 22.124 15.895 1.00 30.80      C
ATOM  1517 CD2 LEU A 215    28.858 24.084 16.093 1.00 30.46      C
ATOM  1518 C   LEU A 215    25.440 21.709 15.191 1.00 31.93      C
ATOM  1519 O   LEU A 215    25.211 22.308 14.145 1.00 32.43      O
ATOM  1520 N   GLN A 216    24.762 20.625 15.551 1.00 33.13      N
ATOM  1521 CA  GLN A 216    23.695 20.108 14.701 1.00 34.56      C
ATOM  1522 CB  GLN A 216    23.435 18.625 14.988 1.00 35.66      C
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Figure 9BB

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ATOM  1523  CG  GLN A 216      24.610  17.700  14.728  1.00 37.89           C
ATOM  1524  CD  GLN A 216      24.241  16.238  14.906  1.00 39.33           C
ATOM  1525  OE1 GLN A 216      23.524  15.665  14.083  1.00 41.09           O
ATOM  1526  NE2 GLN A 216      24.717  15.629  15.988  1.00 39.66           N
ATOM  1527  C   GLN A 216      22.406  20.888  14.939  1.00 34.80           C
ATOM  1528  O   GLN A 216      21.569  21.014  14.047  1.00 35.06           O
ATOM  1529  N   VAL A 217      22.258  21.416  16.148  1.00 34.71           N
ATOM  1530  CA  VAL A 217      21.064  22.156  16.531  1.00 35.07           C
ATOM  1531  CB  VAL A 217      20.710  21.866  18.016  1.00 35.06           C
ATOM  1532  CG1 VAL A 217      19.504  22.685  18.451  1.00 35.49           C
ATOM  1533  CG2 VAL A 217      20.435  20.390  18.192  1.00 35.11           C
ATOM  1534  C   VAL A 217      21.164  23.664  16.336  1.00 35.24           C
ATOM  1535  O   VAL A 217      20.199  24.304  15.925  1.00 34.92           O
ATOM  1536  N   LEU A 218      22.326  24.233  16.640  1.00 35.48           N
ATOM  1537  CA  LEU A 218      22.520  25.674  16.511  1.00 35.98           C
ATOM  1538  CB  LEU A 218      23.837  26.097  17.175  1.00 35.20           C
ATOM  1539  CG  LEU A 218      23.954  25.958  18.699  1.00 34.74           C
ATOM  1540  CD1 LEU A 218      25.415  26.086  19.099  1.00 33.85           C
ATOM  1541  CD2 LEU A 218      23.107  27.018  19.395  1.00 34.29           C
ATOM  1542  C   LEU A 218      22.520  26.143  15.059  1.00 36.85           C
ATOM  1543  O   LEU A 218      22.923  25.408  14.154  1.00 36.56           O
ATOM  1544  N   PRO A 219      22.062  27.382  14.819  1.00 37.78           N
ATOM  1545  CD  PRO A 219      21.542  28.360  15.788  1.00 38.25           C
ATOM  1546  CA  PRO A 219      22.026  27.929  13.461  1.00 38.69           C
ATOM  1547  CB  PRO A 219      21.507  29.354  13.664  1.00 38.57           C
ATOM  1548  CG  PRO A 219      21.840  29.660  15.088  1.00 38.75           C
ATOM  1549  C   PRO A 219      23.390  27.895  12.785  1.00 39.23           C
ATOM  1550  O   PRO A 219      24.422  28.136  13.419  1.00 39.41           O
ATOM  1551  N   GLU A 220      23.381  27.591  11.494  1.00 39.72           N
ATOM  1552  CA  GLU A 220      24.600  27.502  10.698  1.00 40.27           C
ATOM  1553  CB  GLU A 220      24.250  27.481   9.207  1.00 41.80           C
ATOM  1554  CG  GLU A 220      22.941  26.777   8.874  1.00 43.87           C
ATOM  1555  CD  GLU A 220      22.413  27.165   7.498  1.00 45.18           C
ATOM  1556  OE1 GLU A 220      23.087  26.854   6.492  1.00 45.89           O
ATOM  1557  OE2 GLU A 220      21.325  27.789   7.425  1.00 45.96           O
ATOM  1558  C   GLU A 220      25.505  28.698  10.972  1.00 39.71           C
ATOM  1559  O   GLU A 220      25.023  29.808  11.211  1.00 40.05           O
ATOM  1560  N   GLY A 221      26.813  28.466  10.946  1.00 38.99           N
ATOM  1561  CA  GLY A 221      27.758  29.547  11.162  1.00 38.23           C
ATOM  1562  C   GLY A 221      28.059  29.947  12.595  1.00 37.79           C
ATOM  1563  O   GLY A 221      28.875  30.842  12.818  1.00 37.76           O
ATOM  1564  N   THR A 222      27.414  29.308  13.566  1.00 36.92           N
ATOM  1565  CA  THR A 222      27.669  29.637  14.967  1.00 36.06           C
ATOM  1566  CB  THR A 222      26.600  29.039  15.911  1.00 36.28           C
ATOM  1567  OG1 THR A 222      25.286  29.441  15.489  1.00 35.84           O
ATOM  1568  CG2 THR A 222      26.836  29.530  17.331  1.00 35.92           C
ATOM  1569  C   THR A 222      29.031  29.082  15.375  1.00 35.26           C
ATOM  1570  O   THR A 222      29.325  27.904  15.159  1.00 35.42           O
ATOM  1571  N   ARG A 223      29.864  29.934  15.962  1.00 33.89           N
ATOM  1572  CA  ARG A 223      31.187  29.515  16.395  1.00 32.73           C
ATOM  1573  CB  ARG A 223      32.213  30.593  16.048  1.00 33.48           C
ATOM  1574  CG  ARG A 223      33.634  30.257  16.448  1.00 34.74           C
ATOM  1575  CD  ARG A 223      34.572  31.304  15.885  1.00 35.80           C
ATOM  1576  NE  ARG A 223      35.976  31.038  16.180  1.00 36.83           N
ATOM  1577  CZ  ARG A 223      36.975  31.735  15.653  1.00 36.90           C
ATOM  1578  NH1 ARG A 223      36.709  32.722  14.808  1.00 37.42           N
ATOM  1579  NH2 ARG A 223      38.229  31.460  15.974  1.00 37.62           N
ATOM  1580  C   ARG A 223      31.204  29.254  17.896  1.00 31.22           C
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Figure 9CC

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ATOM  1581  O   ARG A 223     30.823  30.118  18.684  1.00 31.14           O
ATOM  1582  N   LEU A 224     31.649  28.063  18.287  1.00 29.77           N
ATOM  1583  CA  LEU A 224     31.714  27.702  19.698  1.00 28.63           C
ATOM  1584  CB  LEU A 224     31.501  26.196  19.885  1.00 28.14           C
ATOM  1585  CG  LEU A 224     30.191  25.617  19.343  1.00 28.31           C
ATOM  1586  CD1 LEU A 224     30.145  24.122  19.618  1.00 27.77           C
ATOM  1587  CD2 LEU A 224     29.011  26.321  19.990  1.00 28.16           C
ATOM  1588  C   LEU A 224     33.074  28.088  20.267  1.00 28.22           C
ATOM  1589  O   LEU A 224     34.113  27.855  19.646  1.00 27.72           O
ATOM  1590  N   VAL A 225     33.055  28.678  21.452  1.00 27.59           N
ATOM  1591  CA  VAL A 225     34.279  29.094  22.114  1.00 27.22           C
ATOM  1592  CB  VAL A 225     34.386  30.638  22.165  1.00 27.19           C
ATOM  1593  CG1 VAL A 225     35.669  31.047  22.875  1.00 27.27           C
ATOM  1594  CG2 VAL A 225     34.346  31.219  20.755  1.00 27.27           C
ATOM  1595  C   VAL A 225     34.315  28.573  23.553  1.00 27.00           C
ATOM  1596  O   VAL A 225     33.343  28.707  24.291  1.00 26.02           O
ATOM  1597  N   ASP A 226     35.427  27.965  23.946  1.00 27.26           N
ATOM  1598  CA  ASP A 226     35.555  27.505  25.319  1.00 28.37           C
ATOM  1599  CB  ASP A 226     35.210  26.008  25.469  1.00 29.27           C
ATOM  1600  CG  ASP A 226     36.130  25.095  24.689  1.00 30.58           C
ATOM  1601  OD1 ASP A 226     37.361  25.166  24.874  1.00 31.43           O
ATOM  1602  OD2 ASP A 226     35.613  24.283  23.891  1.00 32.27           O
ATOM  1603  C   ASP A 226     36.952  27.818  25.835  1.00 28.68           C
ATOM  1604  O   ASP A 226     37.767  28.418  25.126  1.00 28.29           O
ATOM  1605  N   SER A 227     37.222  27.409  27.067  1.00 29.15           N
ATOM  1606  CA  SER A 227     38.493  27.693  27.730  1.00 30.16           C
ATOM  1607  CB  SER A 227     38.212  28.003  29.200  1.00 30.84           C
ATOM  1608  OG  SER A 227     37.330  29.105  29.315  1.00 33.08           O
ATOM  1609  C   SER A 227     39.568  26.613  27.662  1.00 29.90           C
ATOM  1610  O   SER A 227     40.696  26.833  28.118  1.00 30.24           O
ATOM  1611  N   GLY A 228     39.221  25.467  27.089  1.00 29.54           N
ATOM  1612  CA  GLY A 228     40.133  24.333  27.004  1.00 29.07           C
ATOM  1613  C   GLY A 228     41.586  24.537  26.605  1.00 29.10           C
ATOM  1614  O   GLY A 228     42.494  24.267  27.400  1.00 28.05           O
ATOM  1615  N   ALA A 229     41.810  24.983  25.368  1.00 28.66           N
ATOM  1616  CA  ALA A 229     43.161  25.208  24.868  1.00 28.46           C
ATOM  1617  CB  ALA A 229     43.113  25.634  23.399  1.00 28.89           C
ATOM  1618  C   ALA A 229     43.900  26.257  25.694  1.00 28.23           C
ATOM  1619  O   ALA A 229     45.095  26.127  25.934  1.00 28.75           O
ATOM  1620  N   ALA A 230     43.191  27.290  26.135  1.00 28.21           N
ATOM  1621  CA  ALA A 230     43.820  28.341  26.937  1.00 28.47           C
ATOM  1622  CB  ALA A 230     42.872  29.512  27.106  1.00 28.62           C
ATOM  1623  C   ALA A 230     44.248  27.821  28.309  1.00 29.04           C
ATOM  1624  O   ALA A 230     45.253  28.281  28.871  1.00 28.26           O
ATOM  1625  N   ILE A 231     43.476  26.874  28.850  1.00 28.95           N
ATOM  1626  CA  ILE A 231     43.785  26.281  30.149  1.00 29.12           C
ATOM  1627  CB  ILE A 231     42.651  25.351  30.636  1.00 29.08           C
ATOM  1628  CG2 ILE A 231     43.053  24.671  31.953  1.00 28.24           C
ATOM  1629  CG1 ILE A 231     41.364  26.152  30.804  1.00 29.21           C
ATOM  1630  CD1 ILE A 231     41.467  27.238  31.820  1.00 28.47           C
ATOM  1631  C   ILE A 231     45.035  25.442  29.986  1.00 29.33           C
ATOM  1632  O   ILE A 231     45.915  25.428  30.850  1.00 29.46           O
ATOM  1633  N   ALA A 232     45.097  24.729  28.870  1.00 29.68           N
ATOM  1634  CA  ALA A 232     46.237  23.884  28.566  1.00 30.26           C
ATOM  1635  CB  ALA A 232     46.030  23.206  27.223  1.00 30.00           C
ATOM  1636  C   ALA A 232     47.493  24.764  28.538  1.00 31.19           C
ATOM  1637  O   ALA A 232     48.487  24.458  29.202  1.00 31.16           O
ATOM  1638  N   ARG A 233     47.437  25.863  27.784  1.00 31.62           N
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Figure 9DD

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ATOM  1639  CA  ARG A 233      48.576  26.776  27.695  1.00 32.55           C
ATOM  1640  CB  ARG A 233      48.273  27.932  26.729  1.00 32.86           C
ATOM  1641  CG  ARG A 233      48.187  27.516  25.259  1.00 32.98           C
ATOM  1642  CD  ARG A 233      48.181  28.745  24.352  1.00 34.06           C
ATOM  1643  NE  ARG A 233      46.982  29.563  24.530  1.00 34.89           N
ATOM  1644  CZ  ARG A 233      45.818  29.316  23.934  1.00 35.40           C
ATOM  1645  NH1 ARG A 233      45.697  28.281  23.115  1.00 35.59           N
ATOM  1646  NH2 ARG A 233      44.770  30.094  24.168  1.00 35.89           N
ATOM  1647  C   ARG A 233      48.952  27.332  29.069  1.00 32.57           C
ATOM  1648  O   ARG A 233      50.129  27.422  29.402  1.00 32.69           O
ATOM  1649  N   ARG A 234      47.957  27.702  29.869  1.00 32.61           N
ATOM  1650  CA  ARG A 234      48.229  28.229  31.206  1.00 32.84           C
ATOM  1651  CB  ARG A 234      46.934  28.713  31.861  1.00 32.78           C
ATOM  1652  CG  ARG A 234      47.107  29.235  33.280  1.00 33.27           C
ATOM  1653  CD  ARG A 234      48.098  30.400  33.357  1.00 33.63           C
ATOM  1654  NE  ARG A 234      48.091  31.010  34.685  1.00 34.67           N
ATOM  1655  CZ  ARG A 234      48.883  32.009  35.060  1.00 34.84           C
ATOM  1656  NH1 ARG A 234      49.759  32.519  34.204  1.00 35.01           N
ATOM  1657  NH2 ARG A 234      48.794  32.502  36.289  1.00 35.15           N
ATOM  1658  C   ARG A 234      48.885  27.155  32.082  1.00 33.23           C
ATOM  1659  O   ARG A 234      49.760  27.458  32.901  1.00 33.10           O
ATOM  1660  N   THR A 235      48.464  25.906  31.897  1.00 32.93           N
ATOM  1661  CA  THR A 235      49.007  24.778  32.652  1.00 33.19           C
ATOM  1662  CB  THR A 235      48.201  23.486  32.368  1.00 32.74           C
ATOM  1663  OG1 THR A 235      46.879  23.637  32.899  1.00 32.01           O
ATOM  1664  CG2 THR A 235      48.867  22.262  33.013  1.00 32.30           C
ATOM  1665  C   THR A 235      50.475  24.564  32.290  1.00 33.74           C
ATOM  1666  O   THR A 235      51.327  24.396  33.170  1.00 33.08           O
ATOM  1667  N   ALA A 236      50.767  24.586  30.993  1.00 34.60           N
ATOM  1668  CA  ALA A 236      52.135  24.415  30.519  1.00 35.65           C
ATOM  1669  CB  ALA A 236      52.163  24.387  28.994  1.00 35.86           C
ATOM  1670  C   ALA A 236      53.021  25.548  31.042  1.00 36.35           C
ATOM  1671  O   ALA A 236      54.180  25.328  31.388  1.00 36.64           O
ATOM  1672  N   TRP A 237      52.480  26.761  31.109  1.00 37.16           N
ATOM  1673  CA  TRP A 237      53.261  27.893  31.599  1.00 38.00           C
ATOM  1674  CB  TRP A 237      52.509  29.208  31.380  1.00 38.98           C
ATOM  1675  CG  TRP A 237      53.355  30.429  31.649  1.00 40.50           C
ATOM  1676  CD2 TRP A 237      53.400  31.199  32.859  1.00 40.98           C
ATOM  1677  CE2 TRP A 237      54.352  32.228  32.667  1.00 41.43           C
ATOM  1678  CE3 TRP A 237      52.730  31.120  34.087  1.00 41.27           C
ATOM  1679  CD1 TRP A 237      54.260  31.006  30.797  1.00 41.31           C
ATOM  1680  NE1 TRP A 237      54.861  32.088  31.402  1.00 41.47           N
ATOM  1681  CZ2 TRP A 237      54.650  33.171  33.659  1.00 41.56           C
ATOM  1682  CZ3 TRP A 237      53.028  32.058  35.075  1.00 41.51           C
ATOM  1683  CH2 TRP A 237      53.980  33.070  34.852  1.00 41.65           C
ATOM  1684  C   TRP A 237      53.573  27.744  33.092  1.00 38.01           C
ATOM  1685  O   TRP A 237      54.687  28.035  33.537  1.00 37.78           O
ATOM  1686  N   LEU A 238      52.585  27.299  33.862  1.00 37.56           N
ATOM  1687  CA  LEU A 238      52.762  27.127  35.299  1.00 37.57           C
ATOM  1688  CB  LEU A 238      51.408  26.902  35.975  1.00 36.67           C
ATOM  1689  CG  LEU A 238      50.478  28.114  35.957  1.00 36.43           C
ATOM  1690  CD1 LEU A 238      49.116  27.731  36.487  1.00 36.24           C
ATOM  1691  CD2 LEU A 238      51.077  29.235  36.794  1.00 36.56           C
ATOM  1692  C   LEU A 238      53.703  25.977  35.622  1.00 37.81           C
ATOM  1693  O   LEU A 238      54.461  26.040  36.591  1.00 37.91           O
ATOM  1694  N   LEU A 239      53.660  24.923  34.819  1.00 38.48           N
ATOM  1695  CA  LEU A 239      54.540  23.791  35.057  1.00 39.58           C
ATOM  1696  CB  LEU A 239      54.163  22.619  34.149  1.00 39.09           C
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Figure 9EE

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ATOM  1697  CG  LEU A 239      52.839  21.921  34.493  1.00 38.87      C
ATOM  1698  CD1 LEU A 239      52.520  20.870  33.447  1.00 38.45      C
ATOM  1699  CD2 LEU A 239      52.936  21.293  35.881  1.00 38.47      C
ATOM  1700  C   LEU A 239      55.979  24.224  34.791  1.00 40.79      C
ATOM  1701  O   LEU A 239      56.927  23.586  35.249  1.00 40.92      O
ATOM  1702  N   GLU A 240      56.129  25.324  34.060  1.00 41.65      N
ATOM  1703  CA  GLU A 240      57.448  25.837  33.719  1.00 42.84      C
ATOM  1704  CB  GLU A 240      57.444  26.409  32.297  1.00 43.65      C
ATOM  1705  CG  GLU A 240      57.275  25.369  31.200  1.00 45.38      C
ATOM  1706  CD  GLU A 240      58.319  24.268  31.280  1.00 46.58      C
ATOM  1707  OE1 GLU A 240      59.529  24.596  31.325  1.00 47.04      O
ATOM  1708  OE2 GLU A 240      57.929  23.076  31.296  1.00 47.22      O
ATOM  1709  C   GLU A 240      57.961  26.905  34.667  1.00 43.09      C
ATOM  1710  O   GLU A 240      59.150  26.944  34.968  1.00 43.08      O
ATOM  1711  N   HIS A 241      57.069  27.767  35.143  1.00 43.49      N
ATOM  1712  CA  HIS A 241      57.486  28.858  36.011  1.00 44.38      C
ATOM  1713  CB  HIS A 241      57.070  30.186  35.364  1.00 45.65      C
ATOM  1714  CG  HIS A 241      57.586  30.367  33.967  1.00 47.27      C
ATOM  1715  CD2 HIS A 241      58.415  29.604  33.215  1.00 47.86      C
ATOM  1716  ND1 HIS A 241      57.237  31.442  33.178  1.00 47.83      N
ATOM  1717  CE1 HIS A 241      57.825  31.332  32.000  1.00 48.31      C
ATOM  1718  NE2 HIS A 241      58.546  30.225  31.996  1.00 48.70      N
ATOM  1719  C   HIS A 241      57.024  28.846  37.473  1.00 44.07      C
ATOM  1720  O   HIS A 241      57.400  29.741  38.232  1.00 44.13      O
ATOM  1721  N   GLU A 242      56.236  27.853  37.886  1.00 43.53      N
ATOM  1722  CA  GLU A 242      55.754  27.839  39.269  1.00 42.98      C
ATOM  1723  CB  GLU A 242      54.421  28.589  39.359  1.00 43.70      C
ATOM  1724  CG  GLU A 242      54.522  30.087  39.173  1.00 44.78      C
ATOM  1725  CD  GLU A 242      53.167  30.759  39.210  1.00 45.69      C
ATOM  1726  OE1 GLU A 242      52.341  30.397  40.081  1.00 45.73      O
ATOM  1727  OE2 GLU A 242      52.930  31.658  38.375  1.00 46.45      O
ATOM  1728  C   GLU A 242      55.578  26.498  39.977  1.00 42.31      C
ATOM  1729  O   GLU A 242      55.680  26.430  41.200  1.00 42.11      O
ATOM  1730  N   ALA A 243      55.306  25.439  39.224  1.00 41.35      N
ATOM  1731  CA  ALA A 243      55.072  24.127  39.820  1.00 40.63      C
ATOM  1732  CB  ALA A 243      54.557  23.163  38.758  1.00 40.62      C
ATOM  1733  C   ALA A 243      56.262  23.498  40.540  1.00 40.38      C
ATOM  1734  O   ALA A 243      57.382  23.480  40.025  1.00 39.78      O
ATOM  1735  N   PRO A 244      56.028  22.970  41.753  1.00 39.91      N
ATOM  1736  CD  PRO A 244      54.781  23.031  42.540  1.00 39.77      C
ATOM  1737  CA  PRO A 244      57.102  22.331  42.518  1.00 39.80      C
ATOM  1738  CB  PRO A 244      56.495  22.194  43.914  1.00 39.91      C
ATOM  1739  CG  PRO A 244      55.026  21.998  43.617  1.00 39.75      C
ATOM  1740  C   PRO A 244      57.415  20.982  41.875  1.00 39.90      C
ATOM  1741  O   PRO A 244      56.603  20.452  41.114  1.00 39.34      O
ATOM  1742  N   ASP A 245      58.588  20.431  42.176  1.00 40.00      N
ATOM  1743  CA  ASP A 245      59.011  19.149  41.615  1.00 40.24      C
ATOM  1744  CB  ASP A 245      60.516  18.947  41.853  1.00 41.09      C
ATOM  1745  CG  ASP A 245      61.071  17.750  41.102  1.00 41.84      C
ATOM  1746  OD1 ASP A 245      62.133  17.226  41.501  1.00 42.48      O
ATOM  1747  OD2 ASP A 245      60.455  17.334  40.100  1.00 42.69      O
ATOM  1748  C   ASP A 245      58.245  17.957  42.193  1.00 40.06      C
ATOM  1749  O   ASP A 245      58.817  17.131  42.907  1.00 40.25      O
ATOM  1750  N   ALA A 246      56.954  17.864  41.882  1.00 39.77      N
ATOM  1751  CA  ALA A 246      56.121  16.765  42.364  1.00 39.54      C
ATOM  1752  CB  ALA A 246      54.836  17.313  42.982  1.00 39.39      C
ATOM  1753  C   ALA A 246      55.796  15.857  41.182  1.00 39.56      C
ATOM  1754  O   ALA A 246      54.964  16.194  40.338  1.00 39.19      O
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Figure 9FF

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ATOM  1755  N   LYS A 247      56.446  14.699  41.129  1.00 39.47           N
ATOM  1756  CA  LYS A 247      56.245  13.771  40.024  1.00 39.58           C
ATOM  1757  CB  LYS A 247      57.416  13.892  39.049  1.00 40.22           C
ATOM  1758  CG  LYS A 247      58.777  13.707  39.705  1.00 41.70           C
ATOM  1759  CD  LYS A 247      59.910  13.916  38.706  1.00 43.00           C
ATOM  1760  CE  LYS A 247      61.266  13.866  39.394  1.00 43.78           C
ATOM  1761  NZ  LYS A 247      61.482  12.561  40.080  1.00 45.10           N
ATOM  1762  C   LYS A 247      56.097  12.317  40.450  1.00 39.34           C
ATOM  1763  O   LYS A 247      56.453  11.941  41.564  1.00 39.51           O
ATOM  1764  N   SER A 248      55.583  11.499  39.539  1.00 38.98           N
ATOM  1765  CA  SER A 248      55.385  10.082  39.793  1.00 38.69           C
ATOM  1766  CB  SER A 248      54.009   9.856  40.435  1.00 38.62           C
ATOM  1767  OG  SER A 248      53.728   8.479  40.587  1.00 38.23           O
ATOM  1768  C   SER A 248      55.487   9.286  38.492  1.00 38.63           C
ATOM  1769  O   SER A 248      55.262   9.820  37.405  1.00 38.34           O
ATOM  1770  N   ALA A 249      55.830   8.007  38.609  1.00 38.50           N
ATOM  1771  CA  ALA A 249      55.941   7.150  37.438  1.00 38.58           C
ATOM  1772  CB  ALA A 249      57.195   6.275  37.536  1.00 38.58           C
ATOM  1773  C   ALA A 249      54.691   6.281  37.308  1.00 38.38           C
ATOM  1774  O   ALA A 249      54.529   5.558  36.326  1.00 38.36           O
ATOM  1775  N   ASP A 250      53.805   6.357  38.299  1.00 38.17           N
ATOM  1776  CA  ASP A 250      52.572   5.576  38.269  1.00 37.75           C
ATOM  1777  CB  ASP A 250      51.765   5.767  39.562  1.00 38.49           C
ATOM  1778  CG  ASP A 250      52.435   5.136  40.773  1.00 39.62           C
ATOM  1779  OD1 ASP A 250      53.432   4.403  40.593  1.00 40.12           O
ATOM  1780  OD2 ASP A 250      51.960   5.365  41.909  1.00 39.88           O
ATOM  1781  C   ASP A 250      51.722   5.995  37.076  1.00 36.87           C
ATOM  1782  O   ASP A 250      51.859   7.106  36.563  1.00 37.25           O
ATOM  1783  N   ALA A 251      50.845   5.100  36.636  1.00 36.01           N
ATOM  1784  CA  ALA A 251      49.971   5.379  35.504  1.00 34.97           C
ATOM  1785  CB  ALA A 251      49.359   4.086  34.990  1.00 35.52           C
ATOM  1786  C   ALA A 251      48.868   6.349  35.918  1.00 33.97           C
ATOM  1787  O   ALA A 251      48.624   6.547  37.107  1.00 33.63           O
ATOM  1788  N   ASN A 252      48.206   6.948  34.933  1.00 32.74           N
ATOM  1789  CA  ASN A 252      47.131   7.894  35.204  1.00 31.53           C
ATOM  1790  CB  ASN A 252      46.550   8.451  33.903  1.00 31.29           C
ATOM  1791  CG  ASN A 252      47.583   9.156  33.059  1.00 31.11           C
ATOM  1792  OD1 ASN A 252      48.532   9.745  33.580  1.00 30.92           O
ATOM  1793  ND2 ASN A 252      47.397   9.118  31.747  1.00 31.17           N
ATOM  1794  C   ASN A 252      46.025   7.202  35.983  1.00 30.57           C
ATOM  1795  O   ASN A 252      45.737   6.032  35.755  1.00 30.37           O
ATOM  1796  N   ILE A 253      45.398   7.929  36.896  1.00 29.76           N
ATOM  1797  CA  ILE A 253      44.331   7.340  37.694  1.00 29.03           C
ATOM  1798  CB  ILE A 253      44.880   6.919  39.080  1.00 29.45           C
ATOM  1799  CG2 ILE A 253      45.374   8.139  39.833  1.00 29.70           C
ATOM  1800  CG1 ILE A 253      43.802   6.198  39.888  1.00 30.29           C
ATOM  1801  CD1 ILE A 253      44.292   5.736  41.244  1.00 31.33           C
ATOM  1802  C   ILE A 253      43.141   8.286  37.875  1.00 28.11           C
ATOM  1803  O   ILE A 253      43.297   9.512  37.893  1.00 27.59           O
ATOM  1804  N   ALA A 254      41.948   7.705  37.979  1.00 26.97           N
ATOM  1805  CA  ALA A 254      40.733   8.479  38.183  1.00 25.96           C
ATOM  1806  CB  ALA A 254      39.685   8.123  37.125  1.00 25.54           C
ATOM  1807  C   ALA A 254      40.200   8.167  39.578  1.00 25.64           C
ATOM  1808  O   ALA A 254      40.217   7.010  40.013  1.00 25.40           O
ATOM  1809  N   PHE A 255      39.749   9.203  40.276  1.00 24.93           N
ATOM  1810  CA  PHE A 255      39.188   9.061  41.619  1.00 25.25           C
ATOM  1811  CB  PHE A 255      39.931   9.936  42.633  1.00 24.82           C
ATOM  1812  CG  PHE A 255      41.278   9.416  43.044  1.00 25.59           C
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Figure 9GG

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ATOM  1813  CD1 PHE A 255      42.399  10.235  42.953  1.00 25.46           C
ATOM  1814  CD2 PHE A 255      41.422   8.132  43.559  1.00 26.01           C
ATOM  1815  CE1 PHE A 255      43.650   9.789  43.368  1.00 26.29           C
ATOM  1816  CE2 PHE A 255      42.671   7.668  43.982  1.00 26.91           C
ATOM  1817  CZ  PHE A 255      43.790   8.500  43.884  1.00 26.72           C
ATOM  1818  C   PHE A 255      37.726   9.503  41.663  1.00 25.33           C
ATOM  1819  O   PHE A 255      37.370  10.562  41.140  1.00 25.42           O
ATOM  1820  N   CYS A 256      36.874   8.698  42.284  1.00 25.82           N
ATOM  1821  CA  CYS A 256      35.482   9.099  42.462  1.00 26.46           C
ATOM  1822  CB  CYS A 256      34.512   8.041  41.920  1.00 27.23           C
ATOM  1823  SG  CYS A 256      34.653   6.407  42.664  1.00 29.02           S
ATOM  1824  C   CYS A 256      35.364   9.237  43.983  1.00 26.79           C
ATOM  1825  O   CYS A 256      36.246   8.775  44.715  1.00 26.33           O
ATOM  1826  N   MET A 257      34.308   9.877  44.475  1.00 27.23           N
ATOM  1827  CA  MET A 257      34.174  10.030  45.924  1.00 27.99           C
ATOM  1828  CB  MET A 257      33.566  11.395  46.270  1.00 28.01           C
ATOM  1829  CG  MET A 257      34.365  12.586  45.730  1.00 28.41           C
ATOM  1830  SD  MET A 257      36.165  12.503  46.030  1.00 29.78           S
ATOM  1831  CE  MET A 257      36.802  12.840  44.372  1.00 29.70           C
ATOM  1832  C   MET A 257      33.343   8.903  46.536  1.00 28.39           C
ATOM  1833  O   MET A 257      33.310   8.733  47.754  1.00 28.39           O
ATOM  1834  N   ALA A 258      32.691   8.128  45.679  1.00 29.08           N
ATOM  1835  CA  ALA A 258      31.880   6.999  46.117  1.00 30.02           C
ATOM  1836  CB  ALA A 258      30.474   7.460  46.494  1.00 29.75           C
ATOM  1837  C   ALA A 258      31.814   6.007  44.969  1.00 30.76           C
ATOM  1838  O   ALA A 258      31.509   6.379  43.837  1.00 30.44           O
ATOM  1839  N   MET A 259      32.111   4.747  45.259  1.00 31.73           N
ATOM  1840  CA  MET A 259      32.084   3.712  44.236  1.00 32.90           C
ATOM  1841  CB  MET A 259      32.945   2.527  44.675  1.00 34.30           C
ATOM  1842  CG  MET A 259      33.303   1.566  43.559  1.00 36.54           C
ATOM  1843  SD  MET A 259      34.242   2.358  42.237  1.00 38.48           S
ATOM  1844  CE  MET A 259      35.844   2.502  42.974  1.00 37.84           C
ATOM  1845  C   MET A 259      30.638   3.283  44.029  1.00 33.14           C
ATOM  1846  O   MET A 259      30.189   2.272  44.569  1.00 33.45           O
ATOM  1847  N   THR A 260      29.912   4.076  43.250  1.00 32.81           N
ATOM  1848  CA  THR A 260      28.509   3.827  42.955  1.00 32.55           C
ATOM  1849  CB  THR A 260      27.706   5.132  42.987  1.00 32.69           C
ATOM  1850  OG1 THR A 260      28.140   5.973  41.907  1.00 32.32           O
ATOM  1851  CG2 THR A 260      27.911   5.857  44.304  1.00 32.38           C
ATOM  1852  C   THR A 260      28.362   3.260  41.551  1.00 32.45           C
ATOM  1853  O   THR A 260      29.311   3.264  40.765  1.00 32.43           O
ATOM  1854  N   PRO A 261      27.165   2.765  41.212  1.00 32.43           N
ATOM  1855  CD  PRO A 261      26.012   2.408  42.064  1.00 32.73           C
ATOM  1856  CA  PRO A 261      27.002   2.227  39.862  1.00 32.04           C
ATOM  1857  CB  PRO A 261      25.559   1.726  39.864  1.00 32.40           C
ATOM  1858  CG  PRO A 261      25.383   1.268  41.293  1.00 32.56           C
ATOM  1859  C   PRO A 261      27.244   3.333  38.835  1.00 31.88           C
ATOM  1860  O   PRO A 261      27.850   3.096  37.796  1.00 31.83           O
ATOM  1861  N   GLY A 262      26.779   4.545  39.139  1.00 31.39           N
ATOM  1862  CA  GLY A 262      26.971   5.660  38.225  1.00 30.93           C
ATOM  1863  C   GLY A 262      28.439   5.941  37.935  1.00 30.03           C
ATOM  1864  O   GLY A 262      28.831   6.103  36.782  1.00 30.46           O
ATOM  1865  N   ALA A 263      29.254   6.003  38.980  1.00 29.43           N
ATOM  1866  CA  ALA A 263      30.678   6.248  38.816  1.00 28.87           C
ATOM  1867  CB  ALA A 263      31.342   6.409  40.178  1.00 28.90           C
ATOM  1868  C   ALA A 263      31.329   5.099  38.052  1.00 28.88           C
ATOM  1869  O   ALA A 263      32.162   5.314  37.170  1.00 28.36           O
ATOM  1870  N   GLU A 264      30.944   3.874  38.396  1.00 28.76           N
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Figure 9HH

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ATOM  1871  CA  GLU A 264      31.505   2.691  37.752  1.00 29.21      C
ATOM  1872  CB  GLU A 264      30.980   1.432  38.457  1.00 29.05      C
ATOM  1873  CG  GLU A 264      31.358   1.396  39.931  1.00 29.36      C
ATOM  1874  CD  GLU A 264      30.506   0.450  40.767  1.00 29.84      C
ATOM  1875  OE1 GLU A 264      29.389   0.097  40.345  1.00 29.77      O
ATOM  1876  OE2 GLU A 264      30.955   0.080  41.870  1.00 30.70      O
ATOM  1877  C   GLU A 264      31.187   2.662  36.258  1.00 29.35      C
ATOM  1878  O   GLU A 264      32.006   2.220  35.451  1.00 29.37      O
ATOM  1879  N   GLN A 265      30.010   3.157  35.892  1.00 29.70      N
ATOM  1880  CA  GLN A 265      29.601   3.179  34.495  1.00 30.44      C
ATOM  1881  CB  GLN A 265      28.137   3.606  34.381  1.00 31.82      C
ATOM  1882  CG  GLN A 265      27.210   2.667  35.117  1.00 35.27      C
ATOM  1883  CD  GLN A 265      25.751   3.021  34.954  1.00 37.03      C
ATOM  1884  OE1 GLN A 265      24.889   2.428  35.607  1.00 39.00      O
ATOM  1885  NE2 GLN A 265      25.459   3.984  34.078  1.00 38.41      N
ATOM  1886  C   GLN A 265      30.474   4.076  33.621  1.00 29.94      C
ATOM  1887  O   GLN A 265      30.392   4.015  32.396  1.00 29.87      O
ATOM  1888  N   LEU A 266      31.299   4.906  34.247  1.00 29.15      N
ATOM  1889  CA  LEU A 266      32.198   5.791  33.506  1.00 29.01      C
ATOM  1890  CB  LEU A 266      32.496   7.055  34.318  1.00 28.73      C
ATOM  1891  CG  LEU A 266      31.367   8.075  34.425  1.00 29.05      C
ATOM  1892  CD1 LEU A 266      31.842   9.274  35.237  1.00 28.78      C
ATOM  1893  CD2 LEU A 266      30.937   8.502  33.024  1.00 28.78      C
ATOM  1894  C   LEU A 266      33.523   5.113  33.169  1.00 28.86      C
ATOM  1895  O   LEU A 266      34.319   5.643  32.386  1.00 28.44      O
ATOM  1896  N   LEU A 267      33.757   3.939  33.751  1.00 28.56      N
ATOM  1897  CA  LEU A 267      35.010   3.232  33.533  1.00 28.80      C
ATOM  1898  CB  LEU A 267      34.943   1.824  34.133  1.00 29.49      C
ATOM  1899  CG  LEU A 267      36.275   1.073  34.136  1.00 29.76      C
ATOM  1900  CD1 LEU A 267      37.305   1.829  34.979  1.00 29.91      C
ATOM  1901  CD2 LEU A 267      36.058  -0.329  34.700  1.00 30.42      C
ATOM  1902  C   LEU A 267      35.483   3.150  32.080  1.00 28.65      C
ATOM  1903  O   LEU A 267      36.609   3.529  31.782  1.00 28.27      O
ATOM  1904  N   PRO A 268      34.635   2.655  31.161  1.00 28.76      N
ATOM  1905  CD  PRO A 268      33.250   2.185  31.327  1.00 29.21      C
ATOM  1906  CA  PRO A 268      35.058   2.559  29.759  1.00 29.10      C
ATOM  1907  CB  PRO A 268      33.849   1.920  29.074  1.00 29.23      C
ATOM  1908  CG  PRO A 268      32.695   2.343  29.937  1.00 29.74      C
ATOM  1909  C   PRO A 268      35.470   3.902  29.135  1.00 29.03      C
ATOM  1910  O   PRO A 268      36.458   3.971  28.408  1.00 28.44      O
ATOM  1911  N   VAL A 269      34.719   4.961  29.422  1.00 29.23      N
ATOM  1912  CA  VAL A 269      35.045   6.283  28.885  1.00 29.50      C
ATOM  1913  CB  VAL A 269      33.888   7.279  29.118  1.00 30.12      C
ATOM  1914  CG1 VAL A 269      34.278   8.681  28.649  1.00 31.29      C
ATOM  1915  CG2 VAL A 269      32.667   6.812  28.338  1.00 31.48      C
ATOM  1916  C   VAL A 269      36.328   6.791  29.536  1.00 29.16      C
ATOM  1917  O   VAL A 269      37.220   7.299  28.852  1.00 29.31      O
ATOM  1918  N   LEU A 270      36.438   6.635  30.853  1.00 28.36      N
ATOM  1919  CA  LEU A 270      37.640   7.062  31.547  1.00 28.07      C
ATOM  1920  CB  LEU A 270      37.531   6.749  33.048  1.00 27.79      C
ATOM  1921  CG  LEU A 270      36.555   7.621  33.858  1.00 27.73      C
ATOM  1922  CD1 LEU A 270      36.423   7.075  35.273  1.00 26.65      C
ATOM  1923  CD2 LEU A 270      37.060   9.062  33.893  1.00 27.37      C
ATOM  1924  C   LEU A 270      38.859   6.358  30.942  1.00 28.42      C
ATOM  1925  O   LEU A 270      39.918   6.968  30.759  1.00 28.07      O
ATOM  1926  N   GLN A 271      38.706   5.075  30.620  1.00 28.62      N
ATOM  1927  CA  GLN A 271      39.803   4.309  30.036  1.00 29.58      C
ATOM  1928  CB  GLN A 271      39.446   2.815  30.009  1.00 29.77      C
```

Figure 9II

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ATOM  1929 CG  GLN A 271    39.562   2.171  31.395  1.00 29.56      C
ATOM  1930 CD  GLN A 271    39.100   0.719  31.441  1.00 30.15      C
ATOM  1931 OE1 GLN A 271    39.476  -0.030  32.346  1.00 30.14      O
ATOM  1932 NE2 GLN A 271    38.276   0.322  30.480  1.00 29.92      N
ATOM  1933 C   GLN A 271    40.154   4.831  28.641  1.00 30.09      C
ATOM  1934 O   GLN A 271    41.333   4.935  28.298  1.00 30.05      O
ATOM  1935 N   ARG A 272    39.139   5.173  27.850  1.00 30.62      N
ATOM  1936 CA  ARG A 272    39.372   5.733  26.519  1.00 32.09      C
ATOM  1937 CB  ARG A 272    38.051   5.959  25.769  1.00 33.56      C
ATOM  1938 CG  ARG A 272    37.497   4.712  25.080  1.00 36.87      C
ATOM  1939 CD  ARG A 272    36.510   5.071  23.966  1.00 39.07      C
ATOM  1940 NE  ARG A 272    35.236   5.575  24.474  1.00 41.31      N
ATOM  1941 CZ  ARG A 272    34.331   4.826  25.101  1.00 42.35      C
ATOM  1942 NH1 ARG A 272    34.557   3.529  25.295  1.00 42.99      N
ATOM  1943 NH2 ARG A 272    33.201   5.372  25.538  1.00 42.53      N
ATOM  1944 C   ARG A 272    40.119   7.066  26.646  1.00 31.71      C
ATOM  1945 O   ARG A 272    40.888   7.441  25.758  1.00 31.85      O
ATOM  1946 N   TYR A 273    39.892   7.775  27.751  1.00 31.12      N
ATOM  1947 CA  TYR A 273    40.560   9.053  27.996  1.00 30.49      C
ATOM  1948 CB  TYR A 273    39.764   9.912  28.988  1.00 30.13      C
ATOM  1949 CG  TYR A 273    38.764  10.843  28.338  1.00 30.08      C
ATOM  1950 CD1 TYR A 273    37.423  10.485  28.209  1.00 30.27      C
ATOM  1951 CE1 TYR A 273    36.506  11.337  27.600  1.00 30.56      C
ATOM  1952 CD2 TYR A 273    39.165  12.084  27.840  1.00 30.11      C
ATOM  1953 CE2 TYR A 273    38.257  12.944  27.231  1.00 30.62      C
ATOM  1954 CZ  TYR A 273    36.932  12.566  27.113  1.00 31.12      C
ATOM  1955 OH  TYR A 273    36.035  13.413  26.506  1.00 31.48      O
ATOM  1956 C   TYR A 273    41.992   8.902  28.510  1.00 30.66      C
ATOM  1957 O   TYR A 273    42.738   9.878  28.577  1.00 30.68      O
ATOM  1958 N   GLY A 274    42.383   7.687  28.879  1.00 30.61      N
ATOM  1959 CA  GLY A 274    43.740   7.489  29.356  1.00 30.77      C
ATOM  1960 C   GLY A 274    43.881   7.150  30.830  1.00 31.11      C
ATOM  1961 O   GLY A 274    44.991   7.138  31.358  1.00 30.91      O
ATOM  1962 N   PHE A 275    42.766   6.888  31.503  1.00 31.47      N
ATOM  1963 CA  PHE A 275    42.810   6.527  32.918  1.00 32.19      C
ATOM  1964 CB  PHE A 275    41.801   7.348  33.728  1.00 31.21      C
ATOM  1965 CG  PHE A 275    42.032   8.831  33.653  1.00 30.69      C
ATOM  1966 CD1 PHE A 275    41.342   9.611  32.729  1.00 30.41      C
ATOM  1967 CD2 PHE A 275    42.970   9.441  34.477  1.00 29.75      C
ATOM  1968 CE1 PHE A 275    41.587  10.983  32.624  1.00 30.10      C
ATOM  1969 CE2 PHE A 275    43.223  10.809  34.382  1.00 30.33      C
ATOM  1970 CZ  PHE A 275    42.529  11.582  33.451  1.00 30.15      C
ATOM  1971 C   PHE A 275    42.471   5.048  33.007  1.00 33.19      C
ATOM  1972 O   PHE A 275    41.321   4.655  32.821  1.00 33.75      O
ATOM  1973 N   GLU A 276    43.484   4.234  33.277  1.00 34.59      N
ATOM  1974 CA  GLU A 276    43.310   2.789  33.361  1.00 36.07      C
ATOM  1975 CB  GLU A 276    44.675   2.103  33.438  1.00 37.83      C
ATOM  1976 CG  GLU A 276    45.583   2.659  34.528  1.00 39.84      C
ATOM  1977 CD  GLU A 276    46.443   1.587  35.173  1.00 41.24      C
ATOM  1978 OE1 GLU A 276    46.984   0.727  34.439  1.00 42.52      O
ATOM  1979 OE2 GLU A 276    46.588   1.607  36.415  1.00 41.91      O
ATOM  1980 C   GLU A 276    42.478   2.336  34.544  1.00 35.79      C
ATOM  1981 O   GLU A 276    41.703   1.381  34.442  1.00 35.99      O
ATOM  1982 N   THR A 277    42.632   3.035  35.662  1.00 35.29      N
ATOM  1983 CA  THR A 277    41.938   2.665  36.885  1.00 35.33      C
ATOM  1984 CB  THR A 277    42.976   2.238  37.953  1.00 35.95      C
ATOM  1985 OG1 THR A 277    43.827   1.222  37.404  1.00 37.35      O
ATOM  1986 CG2 THR A 277    42.292   1.707  39.198  1.00 36.44      C
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Figure 9JJ

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ATOM  1987 C   THR A 277    41.056  3.753 37.487 1.00 34.38      C
ATOM  1988 O   THR A 277    41.325  4.946 37.339 1.00 33.90      O
ATOM  1989 N   LEU A 278    39.999  3.309 38.162 1.00 33.42      N
ATOM  1990 CA  LEU A 278    39.063  4.180 38.860 1.00 32.84      C
ATOM  1991 CB  LEU A 278    37.660  4.078 38.261 1.00 32.25      C
ATOM  1992 CG  LEU A 278    36.557  4.754 39.080 1.00 31.65      C
ATOM  1993 CD1 LEU A 278    36.739  6.269 39.067 1.00 31.85      C
ATOM  1994 CD2 LEU A 278    35.204  4.385 38.506 1.00 32.00      C
ATOM  1995 C   LEU A 278    39.029  3.683 40.301 1.00 32.90      C
ATOM  1996 O   LEU A 278    38.696  2.523 40.551 1.00 32.50      O
ATOM  1997 N   GLU A 279    39.390  4.549 41.242 1.00 32.79      N
ATOM  1998 CA  GLU A 279    39.390  4.191 42.657 1.00 33.18      C
ATOM  1999 CB  GLU A 279    40.821  4.141 43.212 1.00 33.85      C
ATOM  2000 CG  GLU A 279    41.704  3.034 42.652 1.00 34.93      C
ATOM  2001 CD  GLU A 279    43.103  3.054 43.243 1.00 35.80      C
ATOM  2002 OE1 GLU A 279    43.990  2.345 42.711 1.00 37.17      O
ATOM  2003 OE2 GLU A 279    43.323  3.773 44.242 1.00 35.89      O
ATOM  2004 C   GLU A 279    38.596  5.205 43.472 1.00 33.21      C
ATOM  2005 O   GLU A 279    38.373  6.340 43.037 1.00 31.95      O
ATOM  2006 N   LYS A 280    38.173  4.786 44.660 1.00 33.51      N
ATOM  2007 CA  LYS A 280    37.438  5.666 45.550 1.00 34.17      C
ATOM  2008 CB  LYS A 280    36.529  4.868 46.489 1.00 34.76      C
ATOM  2009 CG  LYS A 280    35.955  5.721 47.620 1.00 35.25      C
ATOM  2010 CD  LYS A 280    34.963  4.950 48.463 1.00 36.16      C
ATOM  2011 CE  LYS A 280    34.444  5.796 49.618 1.00 36.76      C
ATOM  2012 NZ  LYS A 280    33.323  5.103 50.330 1.00 37.23      N
ATOM  2013 C   LYS A 280    38.437  6.456 46.382 1.00 34.45      C
ATOM  2014 O   LYS A 280    39.405  5.901 46.896 1.00 34.38      O
ATOM  2015 N   LEU A 281    38.204  7.756 46.503 1.00 34.75      N
ATOM  2016 CA  LEU A 281    39.079  8.605 47.293 1.00 35.65      C
ATOM  2017 CB  LEU A 281    39.370  9.908 46.550 1.00 35.08      C
ATOM  2018 CG  LEU A 281    40.280 10.898 47.278 1.00 34.82      C
ATOM  2019 CD1 LEU A 281    41.691 10.337 47.360 1.00 34.07      C
ATOM  2020 CD2 LEU A 281    40.273 12.230 46.537 1.00 34.40      C
ATOM  2021 C   LEU A 281    38.392  8.920 48.618 1.00 36.70      C
ATOM  2022 O   LEU A 281    37.230  9.325 48.635 1.00 36.57      O
ATOM  2023 N   ALA A 282    39.105  8.726 49.722 1.00 37.88      N
ATOM  2024 CA  ALA A 282    38.551  9.008 51.045 1.00 39.41      C
ATOM  2025 CB  ALA A 282    39.297  8.204 52.111 1.00 39.19      C
ATOM  2026 C   ALA A 282    38.687 10.501 51.327 1.00 40.14      C
ATOM  2027 O   ALA A 282    39.798 11.023 51.394 1.00 40.34      O
ATOM  2028 N   VAL A 283    37.556 11.179 51.500 1.00 41.23      N
ATOM  2029 CA  VAL A 283    37.550 12.617 51.757 1.00 42.40      C
ATOM  2030 CB  VAL A 283    36.640 13.340 50.746 1.00 42.15      C
ATOM  2031 CG1 VAL A 283    36.654 14.834 51.008 1.00 42.12      C
ATOM  2032 CG2 VAL A 283    37.097 13.037 49.330 1.00 42.22      C
ATOM  2033 C   VAL A 283    37.073 12.974 53.168 1.00 43.56      C
ATOM  2034 O   VAL A 283    36.188 12.315 53.718 1.00 43.82      O
ATOM  2035 N   LEU A 284    37.658 14.025 53.743 1.00 44.69      N
ATOM  2036 CA  LEU A 284    37.290 14.488 55.084 1.00 45.88      C
ATOM  2037 CB  LEU A 284    38.534 14.635 55.968 1.00 46.17      C
ATOM  2038 CG  LEU A 284    39.537 13.487 56.073 1.00 46.66      C
ATOM  2039 CD1 LEU A 284    40.567 13.830 57.143 1.00 46.97      C
ATOM  2040 CD2 LEU A 284    38.822 12.191 56.420 1.00 46.95      C
ATOM  2041 C   LEU A 284    36.591 15.844 55.006 1.00 46.59      C
ATOM  2042 O   LEU A 284    36.980 16.790 55.699 1.00 47.10      O
ATOM  2043 N   GLY A 285    35.567 15.945 54.165 1.00 47.04      N
ATOM  2044 CA  GLY A 285    34.858 17.204 54.025 1.00 47.76      C
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Figure 9KK

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ATOM  2045  C   GLY A 285      33.866  17.240  52.875  1.00 47.90           C
ATOM  2046  O   GLY A 285      32.783  17.840  53.035  1.00 48.58           O
ATOM  2047  OXT GLY A 285      34.176  16.690  51.803  1.00 48.12           O
ATOM  2058  N1  UMA G   1      41.035  30.895  30.822  1.00 29.94           N
ATOM  2059  C2  UMA G   1      40.620  30.440  32.173  1.00 29.32           C
ATOM  2060  N3  UMA G   1      41.658  30.174  33.053  1.00 29.55           N
ATOM  2061  C4  UMA G   1      43.027  30.300  32.772  1.00 29.59           C
ATOM  2062  C5  UMA G   1      43.381  30.771  31.368  1.00 29.56           C
ATOM  2063  C6  UMA G   1      42.392  31.034  30.490  1.00 29.26           C
ATOM  2064  O2  UMA G   1      39.456  30.295  32.514  1.00 29.70           O
ATOM  2065  O4  UMA G   1      43.849  30.029  33.635  1.00 30.57           O
ATOM  2066  C31 UMA G   1      39.920  31.186  29.853  1.00 29.97           C
ATOM  2067  C32 UMA G   1      39.372  32.587  30.063  1.00 30.33           C
ATOM  2068  O32 UMA G   1      37.898  32.677  29.950  1.00 29.77           O
ATOM  2069  C33 UMA G   1      40.048  33.494  29.089  1.00 30.56           C
ATOM  2070  C34 UMA G   1      40.197  32.516  27.939  1.00 31.30           C
ATOM  2071  O34 UMA G   1      40.333  31.219  28.508  1.00 30.67           O
ATOM  2072  O33 UMA G   1      39.089  34.568  28.897  1.00 31.06           O
ATOM  2073  C35 UMA G   1      41.382  32.735  27.086  1.00 31.78           C
ATOM  2074  O35 UMA G   1      42.506  32.919  27.871  1.00 33.40           O
ATOM  2075  PA  UMA G   1      43.918  33.371  27.296  1.00 34.79           P
ATOM  2076  O1A UMA G   1      44.873  32.987  28.345  1.00 34.47           O
ATOM  2077  O2A UMA G   1      44.116  32.774  26.015  1.00 33.73           O
ATOM  2078  O3A UMA G   1      43.778  34.985  27.253  1.00 35.18           O
ATOM  2079  PB  UMA G   1      42.692  36.010  27.815  1.00 37.02           P
ATOM  2080  O1B UMA G   1      41.390  35.816  27.213  1.00 36.86           O
ATOM  2081  O2B UMA G   1      43.287  37.349  27.763  1.00 37.25           O
ATOM  2082  O1' UMA G   1      42.711  35.593  29.403  1.00 37.25           O
ATOM  2083  C1' UMA G   1      43.283  36.339  30.478  1.00 37.93           C
ATOM  2084  C2' UMA G   1      43.951  35.442  31.486  1.00 38.46           C
ATOM  2085  N2' UMA G   1      45.067  34.682  30.893  1.00 38.63           N
ATOM  2086  C7' UMA G   1      46.346  34.910  31.235  1.00 39.00           C
ATOM  2087  O7' UMA G   1      46.649  35.638  32.176  1.00 39.50           O
ATOM  2088  C8' UMA G   1      47.443  34.229  30.444  1.00 39.26           C
ATOM  2089  C3' UMA G   1      42.883  34.508  32.080  1.00 38.65           C
ATOM  2090  O3' UMA G   1      43.460  33.671  33.140  1.00 39.05           O
ATOM  2091  C4' UMA G   1      41.697  35.312  32.664  1.00 38.99           C
ATOM  2092  O4' UMA G   1      40.704  34.446  33.176  1.00 39.14           O
ATOM  2093  C5' UMA G   1      41.102  36.223  31.586  1.00 39.08           C
ATOM  2094  O5' UMA G   1      42.179  37.085  31.056  1.00 38.34           O
ATOM  2095  C6' UMA G   1      40.020  37.154  32.103  1.00 39.49           C
ATOM  2096  O6' UMA G   1      40.509  37.913  33.199  1.00 40.33           O
ATOM  2097  C18 UMA G   1      44.249  34.079  34.286  1.00 39.32           C
ATOM  2098  C19 UMA G   1      43.455  34.233  35.541  1.00 39.68           C
ATOM  2099  O18 UMA G   1      43.782  35.035  36.398  1.00 40.46           O
ATOM  2100  C20 UMA G   1      45.493  33.170  34.364  1.00 39.34           C
ATOM  2101  N4  UMA G   1      42.384  33.428  35.636  1.00 39.52           N
ATOM  2102  C21 UMA G   1      41.528  33.276  36.821  1.00 39.62           C
ATOM  2103  C22 UMA G   1      42.290  32.995  38.151  1.00 39.22           C
ATOM  2104  O19 UMA G   1      43.372  32.371  38.070  1.00 39.54           O
ATOM  2105  O20 UMA G   1      41.806  33.412  39.234  1.00 39.22           O
ATOM  2106  C23 UMA G   1      40.511  32.156  36.571  1.00 39.39           C
ATOM  2107  OH2 WAT S   1      28.597  26.858  34.170  1.00 35.33           O
ATOM  2108  OH2 WAT S   2      39.874  15.622  52.951  1.00 27.02           O
ATOM  2109  OH2 WAT S   3      47.806  29.582  41.793  1.00 26.82           O
ATOM  2110  OH2 WAT S   4      32.712  12.071  49.955  1.00 33.48           O
ATOM  2111  OH2 WAT S   5      34.388  29.141  28.290  1.00 23.66           O
ATOM  2112  OH2 WAT S   6      29.860  12.057  36.929  1.00 28.75           O
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Figure 9LL

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ATOM  2113 OH2 WAT S  7    18.596 31.078 31.314 1.00 34.56      O
ATOM  2114 OH2 WAT S  8    43.746 30.135 36.454 1.00 31.70      O
ATOM  2115 OH2 WAT S  9    40.710 28.228 24.786 1.00 32.34      O
ATOM  2116 OH2 WAT S 10    40.249 20.233 54.144 1.00 31.31      O
ATOM  2117 OH2 WAT S 11    50.729 22.205 49.175 1.00 29.78      O
ATOM  2118 OH2 WAT S 12    36.244 25.185 28.517 1.00 31.80      O
ATOM  2119 OH2 WAT S 13    29.586  1.690 31.020 1.00 35.67      O
ATOM  2120 OH2 WAT S 14    27.347  8.426 41.609 1.00 33.85      O
ATOM  2121 OH2 WAT S 15    37.753 30.653 48.262 1.00 31.49      O
ATOM  2122 OH2 WAT S 16    39.852  0.508 38.143 1.00 34.51      O
ATOM  2123 OH2 WAT S 17    49.787 10.549 30.555 1.00 37.19      O
ATOM  2124 OH2 WAT S 18    48.590 27.775 45.618 1.00 37.05      O
ATOM  2125 OH2 WAT S 19    46.426 30.341 36.837 1.00 31.78      O
ATOM  2126 OH2 WAT S 20    26.420 26.789 43.445 1.00 49.61      O
ATOM  2127 OH2 WAT S 21    46.268 30.739 29.048 1.00 36.68      O
ATOM  2128 OH2 WAT S 22    51.867 28.804 43.136 1.00 49.35      O
ATOM  2129 OH2 WAT S 23    36.825 15.509 25.141 1.00 33.48      O
ATOM  2130 OH2 WAT S 24    33.895 12.303 25.137 1.00 32.90      O
ATOM  2131 OH2 WAT S 25    36.781 35.492 29.625 1.00 32.04      O
ATOM  2132 OH2 WAT S 26    33.992 25.683 29.926 1.00 34.00      O
ATOM  2133 OH2 WAT S 27    24.645 23.077 49.434 1.00 37.03      O
ATOM  2134 OH2 WAT S 28    37.658 21.847 53.629 1.00 28.23      O
ATOM  2135 OH2 WAT S 29    43.589 10.679 50.593 1.00 35.31      O
ATOM  2136 OH2 WAT S 30    23.719 24.494 52.323 1.00 35.79      O
ATOM  2137 OH2 WAT S 31    39.337 10.396 24.048 1.00 52.48      O
ATOM  2138 OH2 WAT S 32    30.718 16.193 20.614 1.00 43.40      O
ATOM  2139 OH2 WAT S 33    54.666  8.115 42.921 1.00 47.38      O
ATOM  2140 OH2 WAT S 34    31.589 30.437 35.873 1.00 47.91      O
ATOM  2141 OH2 WAT S 35    50.340 32.089 31.165 1.00 41.42      O
ATOM  2142 OH2 WAT S 36    52.796 22.874 51.515 1.00 43.37      O
ATOM  2143 OH2 WAT S 37    55.373 22.792 30.536 1.00 57.15      O
ATOM  2144 OH2 WAT S 38    39.463 35.817 35.231 1.00 32.47      O
ATOM  2145 OH2 WAT S 39    16.092 27.159 27.724 1.00 37.21      O
ATOM  2146 OH2 WAT S 40    25.640 24.780 14.005 1.00 45.10      O
ATOM  2147 OH2 WAT S 41    50.761  2.536 38.098 1.00 52.36      O
ATOM  2148 OH2 WAT S 42    18.634 34.668 30.052 1.00 43.13      O
ATOM  2149 OH2 WAT S 43    38.535 -2.076 28.925 1.00 32.09      O
ATOM  2150 OH2 WAT S 44    13.196 24.012 19.544 1.00 39.80      O
ATOM  2151 OH2 WAT S 45    31.357 26.426 13.729 1.00 42.37      O
ATOM  2152 OH2 WAT S 46    52.281 28.184 27.760 1.00 36.04      O
ATOM  2153 OH2 WAT S 47    46.418 33.201 38.411 1.00 44.49      O
ATOM  2154 OH2 WAT S 48    53.339 19.767 45.907 1.00 33.06      O
ATOM  2155 OH2 WAT S 49    46.967 16.612 52.076 1.00 30.83      O
ATOM  2156 OH2 WAT S 50    36.971 22.531 27.836 1.00 27.70      O
ATOM  2157 OH2 WAT S 51    34.404 33.315 13.713 1.00 63.94      O
ATOM  2158 OH2 WAT S 52    25.500 12.910 42.366 1.00 44.85      O
ATOM  2159 OH2 WAT S 53    41.068 33.656 19.666 1.00 61.38      O
ATOM  2160 OH2 WAT S 54    47.085 26.379 21.851 1.00 40.28      O
ATOM  2161 OH2 WAT S 55    20.530 37.341 28.713 1.00 42.17      O
ATOM  2162 OH2 WAT S 56    45.303 21.686 23.767 1.00 31.71      O
ATOM  2163 OH2 WAT S 57    32.171  3.766 47.945 1.00 39.12      O
ATOM  2164 OH2 WAT S 58    29.040 34.613 43.652 1.00 54.88      O
ATOM  2165 OH2 WAT S 59    63.169 17.639 43.696 1.00 51.86      O
ATOM  2166 OH2 WAT S 60    17.466 39.005 16.986 1.00 43.71      O
ATOM  2167 OH2 WAT S 61    31.214  5.360 30.303 1.00 35.40      O
ATOM  2168 OH2 WAT S 62    32.083 34.301 14.884 1.00 43.78      O
ATOM  2169 OH2 WAT S 63    56.027 25.650 46.067 1.00 55.28      O
ATOM  2170 OH2 WAT S 64    49.021 30.852 29.187 1.00 36.47      O
```

Figure 9MM

```
ATOM  2171 OH2 WAT S  65      23.639  30.939  17.071  1.00 45.30           O
ATOM  2172 OH2 WAT S  66      37.468  39.280  36.056  1.00 51.85           O
ATOM  2173 OH2 WAT S  67      36.224  28.879  18.295  1.00 42.91           O
ATOM  2174 OH2 WAT S  68      24.175  22.019  37.073  1.00 26.31           O
ATOM  2175 OH2 WAT S  69      22.152  26.896  48.344  1.00 61.11           O
ATOM  2176 OH2 WAT S  70      48.970   6.753  46.837  1.00 48.46           O
ATOM  2177 OH2 WAT S  71      42.273  27.745  52.837  1.00 33.63           O
ATOM  2178 OH2 WAT S  72      53.543  28.612  47.788  1.00 36.22           O
ATOM  2179 OH2 WAT S  73       8.907  23.447  21.629  1.00 50.44           O
ATOM  2180 OH2 WAT S  74      34.479  41.295  17.726  1.00 40.28           O
ATOM  2181 OH2 WAT S  75      34.584  20.083  21.656  1.00 47.04           O
ATOM  2182 OH2 WAT S  76      48.365   7.218  39.795  1.00 37.47           O
ATOM  2183 OH2 WAT S  77      17.856  23.193  14.949  1.00 36.50           O
ATOM  2184 OH2 WAT S  78      22.607  24.686  38.024  1.00 40.25           O
ATOM  2185 OH2 WAT S  79      21.034  18.474  37.563  1.00 57.62           O
ATOM  2186 OH2 WAT S  80      52.538   9.289  46.345  1.00 43.42           O
ATOM  2187 OH2 WAT S  81      29.673  13.056  39.115  1.00 28.10           O
ATOM  2188 OH2 WAT S  82      25.423  30.052  47.729  1.00 43.44           O
ATOM  2189 OH2 WAT S  83      27.721  18.627  14.255  1.00 44.64           O
ATOM  2190 OH2 WAT S  84      59.509  32.103  35.721  1.00 63.08           O
ATOM  2191 OH2 WAT S  85      44.482  33.024  48.358  1.00 36.03           O
ATOM  2192 OH2 WAT S  86      41.973   7.788  49.345  1.00 50.35           O
ATOM  2193 OH2 WAT S  87      37.663  22.110  25.265  1.00 41.24           O
ATOM  2194 OH2 WAT S  88      25.957  12.097  36.912  1.00 36.00           O
ATOM  2195 OH2 WAT S  89      30.437  33.017  13.345  1.00 48.23           O
ATOM  2196 OH2 WAT S  90      37.438  31.243  38.851  1.00 49.55           O
ATOM  2197 OH2 WAT S  91      19.458  34.402  26.135  1.00 43.19           O
ATOM  2198 OH2 WAT S  92      58.475  14.110  43.025  1.00 52.43           O
ATOM  2199 OH2 WAT S  93      22.370  12.343  33.413  1.00 38.81           O
ATOM  2200 OH2 WAT S  94      40.451  32.550  14.618  1.00 58.82           O
ATOM  2201 OH2 WAT S  95      54.156  16.243  28.025  1.00 48.89           O
ATOM  2202 OH2 WAT S  96      12.252  20.214  20.621  1.00 44.94           O
ATOM  2203 OH2 WAT S  97      23.229  23.360  11.991  1.00 68.77           O
ATOM  2204 OH2 WAT S  98      13.653  34.410  21.575  1.00 50.48           O
ATOM  2205 OH2 WAT S  99      29.882  16.048  51.774  1.00 53.76           O
ATOM  2206 OH2 WAT S 100      34.851   9.916  49.548  1.00 36.26           O
ATOM  2207 OH2 WAT S 101      19.731  39.777  18.001  1.00 49.92           O
ATOM  2208 OH2 WAT S 102      32.811  27.414  53.799  1.00 52.41           O
ATOM  2209 OH2 WAT S 103      54.958  10.260  45.018  1.00 61.62           O
ATOM  2210 OH2 WAT S 104      26.795   8.100  24.207  1.00 39.76           O
ATOM  2211 OH2 WAT S 105      39.473  25.414  23.627  1.00 33.71           O
ATOM  2212 OH2 WAT S 106      42.444  29.282  22.951  1.00 55.44           O
ATOM  2213 OH2 WAT S 107      54.310   2.465  42.338  1.00 81.43           O
ATOM  2214 OH2 WAT S 108      32.145  22.002  57.937  1.00 69.67           O
ATOM  2215 OH2 WAT S 109      41.182  36.953  24.858  1.00 30.32           O
ATOM  2216 OH2 WAT S 110      51.408  18.218  47.152  1.00 39.60           O
ATOM  2217 OH2 WAT S 111      31.229  18.063  15.169  1.00 58.09           O
ATOM  2218 OH2 WAT S 112      47.275  32.201  26.136  1.00 75.84           O
ATOM  2219 OH2 WAT S 113      48.484  -3.729  34.355  1.00 49.03           O
ATOM  2220 OH2 WAT S 114      17.441  23.890  30.338  1.00 38.38           O
ATOM  2221 OH2 WAT S 115      23.853  34.456  13.715  1.00 61.47           O
ATOM  2222 OH2 WAT S 116      22.764  12.193  26.654  1.00 52.95           O
ATOM  2223 OH2 WAT S 117      23.980  15.802  45.364  1.00 50.14           O
ATOM  2224 OH2 WAT S 118      35.972  34.774  45.163  1.00 60.33           O
ATOM  2225 OH2 WAT S 119      37.807  19.398  24.708  1.00 61.62           O
ATOM  2226 OH2 WAT S 120      18.366  12.430  18.822  1.00 41.37           O
ATOM  2227 OH2 WAT S 121      28.690  28.104  42.174  1.00 64.02           O
ATOM  2228 OH2 WAT S 122      49.307   6.503  32.285  1.00 36.36           O
```

Figure 9NN

```
ATOM  2229  OH2 WAT S 123     43.722   4.110  29.378  1.00 44.89           O
ATOM  2230  OH2 WAT S 124     26.343  29.966   7.876  1.00 62.82           O
ATOM  2231  OH2 WAT S 125     16.563  15.951  28.970  1.00 51.98           O
ATOM  2232  OH2 WAT S 126     20.175  23.841  38.565  1.00 55.56           O
ATOM  2233  OH2 WAT S 127     20.576  26.542  40.567  1.00 46.61           O
ATOM  2234  OH2 WAT S 128     40.494  17.605  54.649  1.00 38.00           O
ATOM  2235  OH2 WAT S 129     32.794  26.121  16.217  1.00 40.24           O
ATOM  2236  OH2 WAT S 130     32.054  30.620  12.330  1.00 41.15           O
ATOM  2237  OH2 WAT S 131     24.132   9.866  33.561  1.00 38.41           O
ATOM  2238  OH2 WAT S 132     39.539  30.733  24.819  1.00 33.26           O
ATOM  2239  OH2 WAT S 133     29.283   9.374  37.492  1.00 32.82           O
ATOM  2240  OH2 WAT S 134     27.129  12.130  39.369  1.00 36.01           O
ATOM  2241  OH2 WAT S 135     16.237  13.797  27.208  1.00 39.89           O
ATOM  2242  OH2 WAT S 136     35.590  17.878  24.571  1.00 35.55           O
ATOM  2243  OH2 WAT S 137     22.902  19.820  36.431  1.00 38.01           O
ATOM  2244  OH2 WAT S 138     52.919  12.766  42.677  1.00 32.51           O
ATOM  2245  OH2 WAT S 139     30.240  31.220  40.494  1.00 52.62           O
ATOM  2246  OH2 WAT S 140     37.369  27.649  21.696  1.00 36.64           O
ATOM  2247  OH2 WAT S 141     42.712   1.260  30.209  1.00 50.21           O
ATOM  2248  OH2 WAT S 142     24.778   5.524  41.136  1.00 37.52           O
ATOM  2249  OH2 WAT S 143     49.022  30.149  44.178  1.00 39.81           O
ATOM  2250  OH2 WAT S 144     44.239  27.252  54.601  1.00 45.46           O
ATOM  2251  OH2 WAT S 145     34.188  24.808  21.734  1.00 47.86           O
ATOM  2252  OH2 WAT S 146     32.237  13.936  23.957  1.00 47.59           O
ATOM  2253  OH2 WAT S 147     24.826  31.905  13.806  1.00 57.46           O
ATOM  2254  OH2 WAT S 148     35.287  19.774  55.093  1.00 53.61           O
ATOM  2255  OH2 WAT S 149     37.524  19.283  55.693  1.00 45.09           O
ATOM  2256  OH2 WAT S 150     35.302   8.641  24.481  1.00 51.58           O
ATOM  2257  OH2 WAT S 151     59.678  21.694  39.012  1.00 57.80           O
ATOM  2258  OH2 WAT S 152     36.143  -0.978  27.333  1.00 48.54           O
ATOM  2259  OH2 WAT S 153     14.265  20.928  14.183  1.00 62.49           O
ATOM  2260  OH2 WAT S 154     23.418  29.667  49.908  1.00 54.71           O
ATOM  2261  OH2 WAT S 155     38.604  24.411  54.120  1.00 52.33           O
ATOM  2262  OH2 WAT S 156     27.339  19.921  12.078  1.00 61.52           O
ATOM  2263  OH2 WAT S 157     55.513  12.418  43.797  1.00 48.44           O
ATOM  2264  OH2 WAT S 158     41.570  30.546  53.130  1.00 44.74           O
ATOM  2265  OH2 WAT S 159     30.332   6.416  25.709  1.00 48.89           O
ATOM  2266  OH2 WAT S 160     39.099  33.676  39.711  1.00 61.97           O
ATOM  2267  OH2 WAT S 161     25.263   8.969  43.752  1.00 53.20           O
ATOM  2268  OH2 WAT S 162     38.420  33.913  42.190  1.00 50.80           O
ATOM  2269  OH2 WAT S 163     41.309  37.709  36.508  1.00 59.09           O
ATOM  2270  OH2 WAT S 164     39.795  36.567  20.290  1.00 53.69           O
ATOM  2271  OH2 WAT S 165     17.433  22.843  32.869  1.00 39.36           O
ATOM  2272  OH2 WAT S 166     37.147   1.819  26.855  1.00 35.01           O
ATOM  2273  OH2 WAT S 167     26.808  29.856  51.140  1.00 34.22           O
ATOM  2274  OH2 WAT S 168     20.735  23.758  11.662  1.00 55.01           O
ATOM  2275  OH2 WAT S 169     37.554  20.226  20.434  1.00 54.40           O
ATOM  2276  OH2 WAT S 170     36.378  37.998  37.846  1.00 58.07           O
ATOM  2277  OH2 WAT S 171     18.421  12.604  25.862  1.00 45.72           O
ATOM  2278  OH2 WAT S 172     51.494  14.522  49.973  1.00 41.63           O
ATOM  2279  OH2 WAT S 173     39.132  29.730  18.357  1.00 56.55           O
ATOM  2280  OH2 WAT S 174     45.973  38.322  32.563  1.00 51.66           O
ATOM  2281  OH2 WAT S 175     51.494  34.523  30.878  1.00 51.26           O
ATOM  2282  OH2 WAT S 176     56.959  19.644  38.366  1.00 45.11           O
ATOM  2283  OH2 WAT S 177     27.770  26.356  13.109  1.00 51.59           O
ATOM  2284  OH2 WAT S 178     39.887  26.852  53.281  1.00 46.00           O
ATOM  2285  OH2 WAT S 179     31.617   7.635  49.956  1.00 42.18           O
ATOM  2286  OH2 WAT S 180     43.461  14.656  22.788  1.00 53.80           O
```

Figure 9OO

```
ATOM  2287  OH2 WAT S 181     39.538  18.123  23.159  1.00 56.96      O
ATOM  2288  OH2 WAT S 182     36.797  22.058  22.239  1.00 50.84      O
ATOM  2289  OH2 WAT S 183     15.670  13.383  19.237  1.00 48.91      O
ATOM  2290  OH2 WAT S 184     40.886  32.074  51.060  1.00 46.64      O
ATOM  2291  OH2 WAT S 185     46.429   3.853  37.759  1.00 47.74      O
ATOM  2292  OH2 WAT S 186     51.828  28.947  45.746  1.00 49.80      O
ATOM  2293  OH2 WAT S 187     37.821  12.326  23.248  1.00 59.05      O
ATOM  2294  OH2 WAT S 188     41.682   4.205  47.107  1.00 54.60      O
ATOM  2295  OH2 WAT S 189     24.396  40.185  10.597  1.00 65.04      O
ATOM  2296  OH2 WAT S 190     60.922   7.799  33.813  1.00 57.91      O
ATOM  2297  OH2 WAT S 191     59.350  17.293  37.717  1.00 60.20      O
ATOM  2298  OH2 WAT S 192     26.261  35.674  43.488  1.00 58.18      O
ATOM  2299  OH2 WAT S 193     32.421  28.845  41.543  1.00 57.00      O
ATOM  2300  OH2 WAT S 194     15.680  35.028  23.064  1.00 64.42      O
ATOM  2301  OH2 WAT S 195     38.794   4.828  49.890  1.00 58.11      O
ATOM  2302  OH2 WAT S 196     31.824  29.606  54.893  1.00 42.20      O
ATOM  2303  OH2 WAT S 197     56.033  18.872  46.171  1.00 43.23      O
ATOM  2304  OH2 WAT S 198      9.962  19.461  22.243  1.00 51.63      O
ATOM  2305  OH2 WAT S 199     18.489  10.150  20.863  1.00 54.24      O
ATOM  2306  OH2 WAT S 200     33.066  12.917  52.359  1.00 57.46      O
ATOM  2307  OH2 WAT S 201     30.483   0.016  45.976  1.00 48.00      O
ATOM  2308  OH2 WAT S 202     24.662  11.625  21.208  1.00 44.16      O
ATOM  2309  OH2 WAT S 203     46.715  24.249  23.656  1.00 41.75      O
ATOM  2310  OH2 WAT S 204     17.418  39.478  23.453  1.00 59.60      O
ATOM  2311  OH2 WAT S 205     36.419  43.376  23.037  1.00 52.17      O
ATOM  2312  OH2 WAT S 206     34.959  24.297  19.008  1.00 56.28      O
ATOM  2313  OH2 WAT S 207     43.180  39.844  30.801  1.00 59.11      O
ATOM  2314  OH2 WAT S 208     42.011   9.023  23.239  1.00 63.89      O
ATOM  2315  OH2 WAT S 209     22.676  12.375  19.314  1.00 53.20      O
ATOM  2316  OH2 WAT S 210     17.558  10.038  24.521  1.00 61.87      O
ATOM  2317  OH2 WAT S 211     48.462   5.142  44.693  1.00 58.47      O
ATOM  2318  OH2 WAT S 212     52.898  16.855  49.469  1.00 50.86      O
ATOM  2319  OH2 WAT S 213     37.726  41.234  24.591  1.00 47.40      O
ATOM  2320  OH2 WAT S 214     35.306   2.409  51.472  1.00 56.00      O
ATOM  2321  OH2 WAT S 215     34.107  13.946  54.277  1.00 59.41      O
ATOM  2322  OH2 WAT S 216     39.426  39.934  35.092  1.00 57.35      O
ATOM  2323  OH2 WAT S 217     49.879  15.750  52.077  1.00 59.87      O
ATOM  2324  OH2 WAT S 218     26.673   9.696  22.177  1.00 55.44      O
ATOM  2325  OH2 WAT S 219     22.122  22.199  39.182  1.00 45.37      O
ATOM  2326  OH2 WAT S 220     44.174   7.424  25.089  1.00 54.13      O
ATOM  2327  OH2 WAT S 221     53.760   5.884  44.382  1.00 54.00      O
END
```

Figure 10A

```
REMARK coordinates from minimization and B-factor refinement
REMARK refinement resolution: 500.0 - 1.9 A
REMARK starting r= 0.2224 free_r= 0.2451
REMARK final   r= 0.2185 free_r= 0.2440
REMARK rmsd bonds= 0.006037  rmsd angles=  1.31354
REMARK B rmsd for bonded mainchain atoms=  0.696  target= 1.5
REMARK B rmsd for bonded sidechain atoms=  0.779  target= 2.0
REMARK B rmsd for angle mainchain atoms=  1.253  target= 2.0
REMARK B rmsd for angle sidechain atoms=  1.286  target= 2.5
REMARK target= mlf  final wa= 0.882454  final rweight=0.367395
REMARK cycles= 1 coordinate steps= 150 B-factor steps= 100
REMARK sg= C222(1) a= 83.05 b= 112.82 c= 74.12 alpha= 90 beta= 90 gamma= 90
REMARK topology file 1  : MSI_CNX_TOPPAR:protein.top
REMARK topology file 2  : gll.top
REMARK topology file 3  : MSI_CNX_TOPPAR:water.top
REMARK topology file 4  : MSI_CNX_TOPPAR:ion.top
REMARK topology file 5  : uma.top
REMARK parameter file 1  : MSI_CNX_TOPPAR:protein_rep.param
REMARK parameter file 2  : gll.par
REMARK parameter file 3  : MSI_CNX_TOPPAR:water_rep.param
REMARK parameter file 4  : MSI_CNX_TOPPAR:ion.param
REMARK parameter file 5  : uma.par
REMARK molecular structure file: automatic
REMARK input coordinates: cns8_reb.pdb
REMARK reflection file= ../../../mosflm_esrf/muri_trn_free_unique.fob
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.9
REMARK initial B-factor correction applied to fobs :
REMARK   B11=   3.991 B22=  -8.126 B33=   4.136
REMARK   B12=   0.000 B13=   0.000 B23=   0.000
REMARK B-factor correction applied to coordinate array B:  -0.648
REMARK bulk solvent: (Mask) density level= 0.373583 e/A^3, B-factor= 48.6342 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range:    27807 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):  1265 (  4.5 % )
REMARK number of reflections rejected:                           0 (  0.0 % )
REMARK total number of reflections used:                     26542 ( 95.5 % )
REMARK number of reflections in working set:                 25198 ( 90.6 % )
REMARK number of reflections in test set:                     1344 (  4.8 % )
CRYST1  83.050  112.820  74.120  90.00  90.00  90.00 C 2 2 21
REMARK FILENAME="refine.pdb"
REMARK DATE:Dec-11-2002  01:22:55      created by user: kemitl
REMARK Written by CNX VERSION:2000
ATOM      1  CB  PRO A  20      59.140  10.232  37.959  1.00 42.27       C
ATOM      2  CG  PRO A  20      60.118   9.060  37.995  1.00 42.63       C
ATOM      3  C   PRO A  20      58.220  11.395  35.947  1.00 41.62       C
ATOM      4  O   PRO A  20      59.154  12.042  35.457  1.00 41.55       O
ATOM      5  N   PRO A  20      59.374   9.210  35.773  1.00 42.45       N
ATOM      6  CD  PRO A  20      60.587   8.879  36.540  1.00 42.74       C
ATOM      7  CA  PRO A  20      58.468  10.041  36.605  1.00 42.13       C
ATOM      8  N   ARG A  21      56.961  11.820  35.938  1.00 40.77       N
ATOM      9  CA  ARG A  21      56.586  13.100  35.341  1.00 39.90       C
ATOM     10  CB  ARG A  21      55.792  12.875  34.053  1.00 41.14       C
ATOM     11  CG  ARG A  21      55.782  11.436  33.550  1.00 43.27       C
ATOM     12  CD  ARG A  21      54.592  10.646  34.098  1.00 44.85       C
ATOM     13  NE  ARG A  21      54.310   9.479  33.264  1.00 46.30       N
ATOM     14  CZ  ARG A  21      53.249   8.687  33.392  1.00 46.83       C
```

Figure 10B

```
ATOM   15 NH1 ARG A 21    52.338  8.918 34.332 1.00 46.85      N
ATOM   16 NH2 ARG A 21    53.095  7.661 32.562 1.00 47.39      N
ATOM   17 C  ARG A 21    55.738 13.891 36.327 1.00 38.37      C
ATOM   18 O  ARG A 21    55.175 13.321 37.261 1.00 38.35      O
ATOM   19 N  PRO A 22    55.635 15.217 36.134 1.00 36.71      N
ATOM   20 CD PRO A 22    56.249 16.056 35.092 1.00 36.55      C
ATOM   21 CA PRO A 22    54.834 16.026 37.053 1.00 35.10      C
ATOM   22 CB PRO A 22    54.956 17.441 36.483 1.00 35.61      C
ATOM   23 CG PRO A 22    55.312 17.226 35.048 1.00 36.83      C
ATOM   24 C  PRO A 22    53.392 15.548 37.177 1.00 33.33      C
ATOM   25 O  PRO A 22    52.737 15.204 36.193 1.00 33.12      O
ATOM   26 N  THR A 23    52.926 15.513 38.416 1.00 31.31      N
ATOM   27 CA THR A 23    51.579 15.073 38.734 1.00 28.82      C
ATOM   28 CB THR A 23    51.528 14.500 40.165 1.00 28.86      C
ATOM   29 OG1 THR A 23    52.345 13.324 40.230 1.00 29.00      O
ATOM   30 CG2 THR A 23    50.096 14.159 40.556 1.00 27.97      C
ATOM   31 C  THR A 23    50.615 16.241 38.626 1.00 27.22      C
ATOM   32 O  THR A 23    50.767 17.256 39.307 1.00 26.28      O
ATOM   33 N  VAL A 24    49.622 16.090 37.760 1.00 26.19      N
ATOM   34 CA VAL A 24    48.623 17.123 37.564 1.00 25.17      C
ATOM   35 CB VAL A 24    48.654 17.655 36.116 1.00 25.46      C
ATOM   36 CG1 VAL A 24    47.488 18.596 35.879 1.00 25.44      C
ATOM   37 CG2 VAL A 24    49.976 18.377 35.867 1.00 25.54      C
ATOM   38 C  VAL A 24    47.222 16.617 37.870 1.00 24.64      C
ATOM   39 O  VAL A 24    46.786 15.593 37.344 1.00 24.53      O
ATOM   40 N  LEU A 25    46.525 17.350 38.728 1.00 23.92      N
ATOM   41 CA LEU A 25    45.163 17.004 39.093 1.00 23.77      C
ATOM   42 CB LEU A 25    44.910 17.283 40.579 1.00 23.48      C
ATOM   43 CG LEU A 25    43.437 17.288 41.007 1.00 24.15      C
ATOM   44 CD1 LEU A 25    42.844 15.882 40.865 1.00 23.60      C
ATOM   45 CD2 LEU A 25    43.322 17.779 42.455 1.00 24.84      C
ATOM   46 C  LEU A 25    44.189 17.840 38.279 1.00 23.16      C
ATOM   47 O  LEU A 25    44.368 19.048 38.143 1.00 22.71      O
ATOM   48 N  VAL A 26    43.177 17.183 37.723 1.00 23.08      N
ATOM   49 CA VAL A 26    42.122 17.867 36.991 1.00 22.84      C
ATOM   50 CB VAL A 26    42.017 17.396 35.525 1.00 23.04      C
ATOM   51 CG1 VAL A 26    40.884 18.138 34.832 1.00 22.64      C
ATOM   52 CG2 VAL A 26    43.346 17.665 34.788 1.00 22.73      C
ATOM   53 C  VAL A 26    40.852 17.482 37.764 1.00 23.16      C
ATOM   54 O  VAL A 26    40.520 16.295 37.876 1.00 23.27      O
ATOM   55 N  PHE A 27    40.172 18.485 38.315 1.00 22.82      N
ATOM   56 CA PHE A 27    38.967 18.277 39.117 1.00 23.33      C
ATOM   57 CB PHE A 27    39.168 18.865 40.518 1.00 23.65      C
ATOM   58 CG PHE A 27    37.902 18.924 41.340 1.00 24.66      C
ATOM   59 CD1 PHE A 27    37.456 17.805 42.042 1.00 24.66      C
ATOM   60 CD2 PHE A 27    37.125 20.078 41.360 1.00 24.42      C
ATOM   61 CE1 PHE A 27    36.253 17.834 42.748 1.00 24.95      C
ATOM   62 CE2 PHE A 27    35.917 20.119 42.063 1.00 24.93      C
ATOM   63 CZ PHE A 27    35.480 18.995 42.756 1.00 25.18      C
ATOM   64 C  PHE A 27    37.687 18.879 38.547 1.00 23.64      C
ATOM   65 O  PHE A 27    37.705 19.941 37.931 1.00 24.06      O
ATOM   66 N  ASP A 28    36.575 18.187 38.773 1.00 23.82      N
ATOM   67 CA ASP A 28    35.253 18.651 38.358 1.00 23.43      C
ATOM   68 CB ASP A 28    34.957 18.343 36.885 1.00 23.14      C
ATOM   69 CG ASP A 28    33.602 18.896 36.443 1.00 23.57      C
ATOM   70 OD1 ASP A 28    32.893 18.244 35.646 1.00 23.23      O
ATOM   71 OD2 ASP A 28    33.239 19.998 36.903 1.00 24.14      O
ATOM   72 C  ASP A 28    34.226 17.924 39.202 1.00 23.59      C
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Figure 10C

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ATOM    73  O   ASP A  28      34.540  16.928  39.856  1.00 23.62           O
ATOM    74  N   SER A  29      32.996  18.421  39.179  1.00 23.49           N
ATOM    75  CA  SER A  29      31.904  17.800  39.913  1.00 23.63           C
ATOM    76  CB  SER A  29      30.717  18.757  39.969  1.00 23.55           C
ATOM    77  OG  SER A  29      30.313  19.099  38.657  1.00 24.80           O
ATOM    78  C   SER A  29      31.500  16.508  39.186  1.00 23.67           C
ATOM    79  O   SER A  29      31.007  15.564  39.804  1.00 23.60           O
ATOM    80  N   GLY A  30      31.721  16.471  37.874  1.00 23.60           N
ATOM    81  CA  GLY A  30      31.377  15.294  37.096  1.00 23.98           C
ATOM    82  C   GLY A  30      32.306  15.003  35.934  1.00 23.76           C
ATOM    83  O   GLY A  30      33.529  14.975  36.099  1.00 24.03           O
ATOM    84  N   VAL A  31      31.737  14.799  34.747  1.00 23.50           N
ATOM    85  CA  VAL A  31      32.536  14.491  33.566  1.00 23.42           C
ATOM    86  CB  VAL A  31      31.753  13.579  32.565  1.00 24.04           C
ATOM    87  CG1 VAL A  31      31.393  12.253  33.231  1.00 24.26           C
ATOM    88  CG2 VAL A  31      30.484  14.277  32.079  1.00 24.22           C
ATOM    89  C   VAL A  31      33.054  15.712  32.792  1.00 23.39           C
ATOM    90  O   VAL A  31      33.948  15.576  31.960  1.00 22.93           O
ATOM    91  N   GLY A  32      32.503  16.892  33.062  1.00 23.03           N
ATOM    92  CA  GLY A  32      32.933  18.083  32.341  1.00 23.53           C
ATOM    93  C   GLY A  32      34.434  18.316  32.374  1.00 23.94           C
ATOM    94  O   GLY A  32      35.018  18.803  31.406  1.00 23.61           O
ATOM    95  N   GLY A  33      35.058  17.971  33.496  1.00 23.88           N
ATOM    96  CA  GLY A  33      36.492  18.149  33.641  1.00 24.00           C
ATOM    97  C   GLY A  33      37.272  17.468  32.537  1.00 24.04           C
ATOM    98  O   GLY A  33      38.347  17.921  32.174  1.00 24.11           O
ATOM    99  N   LEU A  34      36.720  16.389  31.990  1.00 24.29           N
ATOM   100  CA  LEU A  34      37.377  15.653  30.923  1.00 24.12           C
ATOM   101  CB  LEU A  34      36.586  14.384  30.589  1.00 24.26           C
ATOM   102  CG  LEU A  34      36.559  13.331  31.703  1.00 24.52           C
ATOM   103  CD1 LEU A  34      35.609  12.209  31.311  1.00 24.48           C
ATOM   104  CD2 LEU A  34      37.969  12.795  31.940  1.00 24.92           C
ATOM   105  C   LEU A  34      37.586  16.474  29.652  1.00 23.95           C
ATOM   106  O   LEU A  34      38.524  16.212  28.907  1.00 24.13           O
ATOM   107  N   SER A  35      36.729  17.461  29.394  1.00 23.76           N
ATOM   108  CA  SER A  35      36.916  18.270  28.191  1.00 24.21           C
ATOM   109  CB  SER A  35      35.694  19.159  27.909  1.00 23.45           C
ATOM   110  OG  SER A  35      35.531  20.175  28.886  1.00 23.98           O
ATOM   111  C   SER A  35      38.173  19.137  28.347  1.00 24.34           C
ATOM   112  O   SER A  35      38.910  19.357  27.383  1.00 24.46           O
ATOM   113  N   VAL A  36      38.416  19.611  29.564  1.00 24.57           N
ATOM   114  CA  VAL A  36      39.582  20.444  29.847  1.00 25.04           C
ATOM   115  CB  VAL A  36      39.445  21.160  31.211  1.00 25.08           C
ATOM   116  CG1 VAL A  36      40.682  22.024  31.482  1.00 25.12           C
ATOM   117  CG2 VAL A  36      38.188  22.020  31.212  1.00 25.41           C
ATOM   118  C   VAL A  36      40.824  19.572  29.863  1.00 25.61           C
ATOM   119  O   VAL A  36      41.869  19.935  29.313  1.00 25.10           O
ATOM   120  N   TYR A  37      40.704  18.407  30.494  1.00 26.15           N
ATOM   121  CA  TYR A  37      41.816  17.478  30.550  1.00 26.62           C
ATOM   122  CB  TYR A  37      41.427  16.236  31.367  1.00 26.04           C
ATOM   123  CG  TYR A  37      42.210  14.999  31.006  1.00 26.11           C
ATOM   124  CD1 TYR A  37      41.696  14.065  30.106  1.00 26.04           C
ATOM   125  CE1 TYR A  37      42.431  12.937  29.737  1.00 26.06           C
ATOM   126  CD2 TYR A  37      43.483  14.777  31.532  1.00 26.28           C
ATOM   127  CE2 TYR A  37      44.227  13.654  31.167  1.00 26.29           C
ATOM   128  CZ  TYR A  37      43.694  12.742  30.274  1.00 26.29           C
ATOM   129  OH  TYR A  37      44.414  11.627  29.922  1.00 26.91           O
ATOM   130  C   TYR A  37      42.243  17.072  29.139  1.00 27.35           C
```

Figure 10D

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ATOM   131  O   TYR A  37      43.431  16.998  28.840  1.00 27.42           O
ATOM   132  N   ASP A  38      41.270  16.815  28.274  1.00 28.14           N
ATOM   133  CA  ASP A  38      41.554  16.403  26.906  1.00 29.79           C
ATOM   134  CB  ASP A  38      40.234  16.233  26.149  1.00 30.37           C
ATOM   135  CG  ASP A  38      40.355  15.321  24.945  1.00 31.87           C
ATOM   136  OD1 ASP A  38      41.285  14.487  24.904  1.00 32.39           O
ATOM   137  OD2 ASP A  38      39.495  15.427  24.039  1.00 32.89           O
ATOM   138  C   ASP A  38      42.472  17.411  26.200  1.00 30.27           C
ATOM   139  O   ASP A  38      43.406  17.018  25.500  1.00 30.51           O
ATOM   140  N   GLU A  39      42.213  18.702  26.399  1.00 30.88           N
ATOM   141  CA  GLU A  39      43.032  19.759  25.799  1.00 32.05           C
ATOM   142  CB  GLU A  39      42.367  21.123  25.992  1.00 32.93           C
ATOM   143  CG  GLU A  39      41.075  21.325  25.219  1.00 35.19           C
ATOM   144  CD  GLU A  39      41.310  21.703  23.766  1.00 36.77           C
ATOM   145  OE1 GLU A  39      40.316  21.968  23.056  1.00 38.63           O
ATOM   146  OE2 GLU A  39      42.481  21.743  23.333  1.00 37.13           O
ATOM   147  C   GLU A  39      44.417  19.786  26.447  1.00 32.29           C
ATOM   148  O   GLU A  39      45.435  19.941  25.772  1.00 31.60           O
ATOM   149  N   ILE A  40      44.454  19.640  27.765  1.00 32.60           N
ATOM   150  CA  ILE A  40      45.726  19.646  28.472  1.00 33.11           C
ATOM   151  CB  ILE A  40      45.517  19.585  29.998  1.00 32.73           C
ATOM   152  CG2 ILE A  40      46.867  19.494  30.709  1.00 32.95           C
ATOM   153  CG1 ILE A  40      44.750  20.824  30.468  1.00 32.28           C
ATOM   154  CD1 ILE A  40      44.401  20.809  31.947  1.00 32.55           C
ATOM   155  C   ILE A  40      46.623  18.486  28.040  1.00 33.95           C
ATOM   156  O   ILE A  40      47.806  18.688  27.753  1.00 33.92           O
ATOM   157  N   ARG A  41      46.072  17.275  27.982  1.00 34.92           N
ATOM   158  CA  ARG A  41      46.872  16.118  27.593  1.00 36.38           C
ATOM   159  CB  ARG A  41      46.114  14.805  27.815  1.00 36.95           C
ATOM   160  CG  ARG A  41      44.970  14.556  26.850  1.00 38.65           C
ATOM   161  CD  ARG A  41      44.714  13.060  26.676  1.00 40.05           C
ATOM   162  NE  ARG A  41      43.499  12.807  25.905  1.00 41.30           N
ATOM   163  CZ  ARG A  41      43.076  11.600  25.541  1.00 41.65           C
ATOM   164  NH1 ARG A  41      43.770  10.518  25.872  1.00 41.91           N
ATOM   165  NH2 ARG A  41      41.952  11.475  24.847  1.00 42.04           N
ATOM   166  C   ARG A  41      47.324  16.188  26.141  1.00 37.23           C
ATOM   167  O   ARG A  41      48.347  15.618  25.780  1.00 36.68           O
ATOM   168  N   HIS A  42      46.554  16.870  25.303  1.00 38.38           N
ATOM   169  CA  HIS A  42      46.935  16.990  23.905  1.00 39.98           C
ATOM   170  CB  HIS A  42      45.803  17.637  23.102  1.00 40.97           C
ATOM   171  CG  HIS A  42      46.096  17.757  21.640  1.00 42.48           C
ATOM   172  CD2 HIS A  42      45.580  17.104  20.571  1.00 43.17           C
ATOM   173  ND1 HIS A  42      47.032  18.634  21.137  1.00 43.19           N
ATOM   174  CE1 HIS A  42      47.080  18.519  19.821  1.00 43.48           C
ATOM   175  NE2 HIS A  42      46.208  17.597  19.452  1.00 43.37           N
ATOM   176  C   HIS A  42      48.207  17.836  23.822  1.00 40.26           C
ATOM   177  O   HIS A  42      49.053  17.625  22.955  1.00 40.52           O
ATOM   178  N   LEU A  43      48.341  18.783  24.747  1.00 40.38           N
ATOM   179  CA  LEU A  43      49.500  19.662  24.795  1.00 40.54           C
ATOM   180  CB  LEU A  43      49.087  21.020  25.372  1.00 40.84           C
ATOM   181  CG  LEU A  43      50.118  22.150  25.372  1.00 40.88           C
ATOM   182  CD1 LEU A  43      50.521  22.468  23.935  1.00 41.44           C
ATOM   183  CD2 LEU A  43      49.533  23.386  26.043  1.00 40.98           C
ATOM   184  C   LEU A  43      50.638  19.065  25.631  1.00 40.74           C
ATOM   185  O   LEU A  43      51.812  19.224  25.299  1.00 40.80           O
ATOM   186  N   LEU A  44      50.284  18.379  26.715  1.00 40.77           N
ATOM   187  CA  LEU A  44      51.263  17.759  27.615  1.00 40.94           C
ATOM   188  CB  LEU A  44      51.281  18.515  28.942  1.00 40.98           C
```

Figure 10E

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ATOM   189  CG  LEU A  44      51.493  20.023  28.814  1.00 40.82           C
ATOM   190  CD1 LEU A  44      51.011  20.721  30.066  1.00 40.73           C
ATOM   191  CD2 LEU A  44      52.964  20.307  28.550  1.00 41.26           C
ATOM   192  C   LEU A  44      50.841  16.310  27.841  1.00 41.15           C
ATOM   193  O   LEU A  44      50.325  15.955  28.903  1.00 41.15           O
ATOM   194  N   PRO A  45      51.075  15.445  26.843  1.00 41.22           N
ATOM   195  CD  PRO A  45      51.677  15.806  25.545  1.00 41.47           C
ATOM   196  CA  PRO A  45      50.725  14.021  26.873  1.00 41.13           C
ATOM   197  CB  PRO A  45      50.900  13.604  25.413  1.00 41.22           C
ATOM   198  CG  PRO A  45      52.040  14.456  24.968  1.00 41.02           C
ATOM   199  C   PRO A  45      51.418  13.044  27.826  1.00 41.10           C
ATOM   200  O   PRO A  45      50.885  11.961  28.077  1.00 41.10           O
ATOM   201  N   ASP A  46      52.576  13.400  28.373  1.00 40.74           N
ATOM   202  CA  ASP A  46      53.280  12.454  29.240  1.00 40.25           C
ATOM   203  CB  ASP A  46      54.765  12.400  28.854  1.00 41.61           C
ATOM   204  CG  ASP A  46      54.974  12.058  27.391  1.00 43.12           C
ATOM   205  OD1 ASP A  46      54.498  10.985  26.956  1.00 43.83           O
ATOM   206  OD2 ASP A  46      55.618  12.863  26.676  1.00 44.38           O
ATOM   207  C   ASP A  46      53.176  12.666  30.749  1.00 38.90           C
ATOM   208  O   ASP A  46      53.812  11.941  31.511  1.00 39.20           O
ATOM   209  N   LEU A  47      52.381  13.636  31.185  1.00 36.81           N
ATOM   210  CA  LEU A  47      52.249  13.907  32.614  1.00 34.74           C
ATOM   211  CB  LEU A  47      51.450  15.194  32.833  1.00 34.94           C
ATOM   212  CG  LEU A  47      51.913  16.438  32.077  1.00 34.69           C
ATOM   213  CD1 LEU A  47      51.018  17.604  32.434  1.00 35.28           C
ATOM   214  CD2 LEU A  47      53.358  16.746  32.428  1.00 35.67           C
ATOM   215  C   LEU A  47      51.564  12.774  33.364  1.00 33.31           C
ATOM   216  O   LEU A  47      50.968  11.881  32.758  1.00 33.06           O
ATOM   217  N   HIS A  48      51.678  12.800  34.689  1.00 31.91           N
ATOM   218  CA  HIS A  48      51.013  11.808  35.530  1.00 30.54           C
ATOM   219  CB  HIS A  48      51.794  11.524  36.814  1.00 30.57           C
ATOM   220  CG  HIS A  48      51.017  10.729  37.822  1.00 30.87           C
ATOM   221  CD2 HIS A  48      50.251   9.620  37.685  1.00 30.97           C
ATOM   222  ND1 HIS A  48      50.986  11.050  39.163  1.00 31.68           N
ATOM   223  CE1 HIS A  48      50.236  10.173  39.808  1.00 31.33           C
ATOM   224  NE2 HIS A  48      49.778   9.295  38.933  1.00 31.22           N
ATOM   225  C   HIS A  48      49.704  12.490  35.900  1.00 29.55           C
ATOM   226  O   HIS A  48      49.668  13.331  36.802  1.00 29.03           O
ATOM   227  N   TYR A  49      48.641  12.139  35.194  1.00 28.24           N
ATOM   228  CA  TYR A  49      47.349  12.754  35.441  1.00 27.76           C
ATOM   229  CB  TYR A  49      46.555  12.878  34.135  1.00 28.09           C
ATOM   230  CG  TYR A  49      47.108  13.881  33.145  1.00 28.48           C
ATOM   231  CD1 TYR A  49      47.890  13.471  32.066  1.00 28.86           C
ATOM   232  CE1 TYR A  49      48.375  14.395  31.124  1.00 29.12           C
ATOM   233  CD2 TYR A  49      46.823  15.242  33.275  1.00 28.88           C
ATOM   234  CE2 TYR A  49      47.301  16.173  32.350  1.00 29.31           C
ATOM   235  CZ  TYR A  49      48.075  15.741  31.275  1.00 29.63           C
ATOM   236  OH  TYR A  49      48.527  16.665  30.353  1.00 29.75           O
ATOM   237  C   TYR A  49      46.477  12.040  36.463  1.00 27.00           C
ATOM   238  O   TYR A  49      46.433  10.808  36.533  1.00 26.57           O
ATOM   239  N   ILE A  50      45.791  12.844  37.259  1.00 25.98           N
ATOM   240  CA  ILE A  50      44.854  12.340  38.243  1.00 24.91           C
ATOM   241  CB  ILE A  50      45.259  12.705  39.682  1.00 24.96           C
ATOM   242  CG2 ILE A  50      44.167  12.253  40.654  1.00 23.79           C
ATOM   243  CG1 ILE A  50      46.598  12.054  40.041  1.00 24.11           C
ATOM   244  CD1 ILE A  50      47.213  12.622  41.313  1.00 24.92           C
ATOM   245  C   ILE A  50      43.560  13.071  37.933  1.00 24.67           C
ATOM   246  O   ILE A  50      43.536  14.305  37.900  1.00 24.39           O
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Figure 10F

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ATOM   247  N  TYR A  51     42.498  12.321  37.671  1.00 24.20      N
ATOM   248  CA  TYR A  51     41.205  12.933  37.413  1.00 24.34      C
ATOM   249  CB  TYR A  51     40.549  12.369  36.148  1.00 24.65      C
ATOM   250  CG  TYR A  51     39.285  13.123  35.766  1.00 25.11      C
ATOM   251  CD1 TYR A  51     38.018  12.626  36.076  1.00 25.28      C
ATOM   252  CE1 TYR A  51     36.860  13.369  35.793  1.00 25.75      C
ATOM   253  CD2 TYR A  51     39.366  14.376  35.157  1.00 25.76      C
ATOM   254  CE2 TYR A  51     38.220  15.122  34.867  1.00 25.82      C
ATOM   255  CZ  TYR A  51     36.974  14.620  35.189  1.00 26.04      C
ATOM   256  OH  TYR A  51     35.856  15.394  34.926  1.00 25.60      O
ATOM   257  C  TYR A  51     40.337  12.612  38.616  1.00 24.47      C
ATOM   258  O  TYR A  51     40.221  11.451  39.014  1.00 24.67      O
ATOM   259  N  ALA A  52     39.740  13.637  39.208  1.00 24.11      N
ATOM   260  CA  ALA A  52     38.878  13.425  40.363  1.00 23.89      C
ATOM   261  CB  ALA A  52     39.533  13.994  41.619  1.00 23.82      C
ATOM   262  C  ALA A  52     37.533  14.090  40.131  1.00 23.96      C
ATOM   263  O  ALA A  52     37.466  15.253  39.723  1.00 23.07      O
ATOM   264  N  PHE A  53     36.461  13.347  40.372  1.00 23.37      N
ATOM   265  CA  PHE A  53     35.132  13.906  40.208  1.00 23.51      C
ATOM   266  CB  PHE A  53     34.474  13.388  38.909  1.00 23.73      C
ATOM   267  CG  PHE A  53     34.310  11.889  38.838  1.00 24.04      C
ATOM   268  CD1 PHE A  53     33.054  11.309  39.007  1.00 23.82      C
ATOM   269  CD2 PHE A  53     35.398  11.066  38.559  1.00 24.45      C
ATOM   270  CE1 PHE A  53     32.882   9.929  38.895  1.00 24.38      C
ATOM   271  CE2 PHE A  53     35.242   9.679  38.445  1.00 24.39      C
ATOM   272  CZ  PHE A  53     33.978   9.111  38.614  1.00 24.35      C
ATOM   273  C  PHE A  53     34.276  13.625  41.444  1.00 23.79      C
ATOM   274  O  PHE A  53     34.305  12.528  42.013  1.00 22.86      O
ATOM   275  N  ASP A  54     33.533  14.642  41.868  1.00 23.79      N
ATOM   276  CA  ASP A  54     32.682  14.541  43.051  1.00 24.06      C
ATOM   277  CB  ASP A  54     32.563  15.916  43.714  1.00 23.89      C
ATOM   278  CG  ASP A  54     31.963  15.840  45.109  1.00 23.89      C
ATOM   279  OD1 ASP A  54     31.577  14.727  45.538  1.00 22.90      O
ATOM   280  OD2 ASP A  54     31.880  16.894  45.772  1.00 23.05      O
ATOM   281  C  ASP A  54     31.289  14.002  42.734  1.00 24.18      C
ATOM   282  O  ASP A  54     30.312  14.750  42.734  1.00 23.82      O
ATOM   283  N  ASN A  55     31.191  12.698  42.488  1.00 24.17      N
ATOM   284  CA  ASN A  55     29.905  12.103  42.170  1.00 25.09      C
ATOM   285  CB  ASN A  55     30.090  10.674  41.631  1.00 25.26      C
ATOM   286  CG  ASN A  55     30.731   9.737  42.639  1.00 25.36      C
ATOM   287  OD1 ASN A  55     31.791  10.028  43.201  1.00 24.79      O
ATOM   288  ND2 ASN A  55     30.092   8.592  42.864  1.00 25.74      N
ATOM   289  C  ASN A  55     28.970  12.110  43.376  1.00 25.56      C
ATOM   290  O  ASN A  55     27.770  11.915  43.226  1.00 25.79      O
ATOM   291  N  VAL A  56     29.520  12.362  44.561  1.00 25.66      N
ATOM   292  CA  VAL A  56     28.731  12.405  45.794  1.00 26.16      C
ATOM   293  CB  VAL A  56     29.642  12.231  47.043  1.00 26.47      C
ATOM   294  CG1 VAL A  56     28.888  12.614  48.320  1.00 26.82      C
ATOM   295  CG2 VAL A  56     30.112  10.785  47.140  1.00 26.75      C
ATOM   296  C  VAL A  56     27.930  13.704  45.950  1.00 26.34      C
ATOM   297  O  VAL A  56     26.779  13.683  46.395  1.00 26.27      O
ATOM   298  N  ALA A  57     28.528  14.831  45.576  1.00 25.69      N
ATOM   299  CA  ALA A  57     27.846  16.106  45.723  1.00 25.62      C
ATOM   300  CB  ALA A  57     28.721  17.072  46.509  1.00 25.61      C
ATOM   301  C  ALA A  57     27.399  16.740  44.405  1.00 25.80      C
ATOM   302  O  ALA A  57     26.813  17.820  44.406  1.00 25.99      O
ATOM   303  N  PHE A  58     27.675  16.079  43.284  1.00 25.66      N
ATOM   304  CA  PHE A  58     27.242  16.595  41.984  1.00 25.94      C
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Figure 10G

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ATOM   305  CB  PHE A  58      27.689  15.659  40.856  1.00 25.77           C
ATOM   306  CG  PHE A  58      27.101  16.006  39.517  1.00 26.33           C
ATOM   307  CD1 PHE A  58      27.725  16.933  38.684  1.00 26.01           C
ATOM   308  CD2 PHE A  58      25.892  15.445  39.112  1.00 26.14           C
ATOM   309  CE1 PHE A  58      27.152  17.300  37.467  1.00 26.79           C
ATOM   310  CE2 PHE A  58      25.308  15.807  37.893  1.00 27.07           C
ATOM   311  CZ  PHE A  58      25.938  16.735  37.071  1.00 27.22           C
ATOM   312  C   PHE A  58      25.714  16.601  42.045  1.00 26.23           C
ATOM   313  O   PHE A  58      25.123  15.651  42.555  1.00 26.27           O
ATOM   314  N   PRO A  59      25.053  17.645  41.507  1.00 26.87           N
ATOM   315  CD  PRO A  59      23.589  17.565  41.316  1.00 27.24           C
ATOM   316  CA  PRO A  59      25.591  18.836  40.838  1.00 27.09           C
ATOM   317  CB  PRO A  59      24.484  19.195  39.850  1.00 27.32           C
ATOM   318  CG  PRO A  59      23.257  18.898  40.647  1.00 27.45           C
ATOM   319  C   PRO A  59      25.902  19.993  41.788  1.00 27.44           C
ATOM   320  O   PRO A  59      25.197  20.214  42.776  1.00 26.87           O
ATOM   321  N   TYR A  60      26.968  20.725  41.476  1.00 28.08           N
ATOM   322  CA  TYR A  60      27.395  21.870  42.277  1.00 29.46           C
ATOM   323  CB  TYR A  60      28.873  22.182  41.988  1.00 28.52           C
ATOM   324  CG  TYR A  60      29.887  21.318  42.725  1.00 27.75           C
ATOM   325  CD1 TYR A  60      29.520  20.113  43.339  1.00 27.37           C
ATOM   326  CE1 TYR A  60      30.475  19.317  44.006  1.00 26.91           C
ATOM   327  CD2 TYR A  60      31.228  21.708  42.794  1.00 27.09           C
ATOM   328  CE2 TYR A  60      32.178  20.932  43.450  1.00 27.19           C
ATOM   329  CZ  TYR A  60      31.802  19.739  44.054  1.00 27.07           C
ATOM   330  OH  TYR A  60      32.758  18.982  44.698  1.00 25.80           O
ATOM   331  C   TYR A  60      26.539  23.119  41.991  1.00 30.92           C
ATOM   332  O   TYR A  60      26.389  23.993  42.849  1.00 30.67           O
ATOM   333  N   GLY A  61      25.981  23.190  40.785  1.00 33.00           N
ATOM   334  CA  GLY A  61      25.165  24.332  40.400  1.00 35.24           C
ATOM   335  C   GLY A  61      24.126  24.770  41.418  1.00 37.04           C
ATOM   336  O   GLY A  61      23.892  25.965  41.601  1.00 37.85           O
ATOM   337  N   GLU A  62      23.512  23.803  42.089  1.00 38.35           N
ATOM   338  CA  GLU A  62      22.479  24.069  43.088  1.00 39.52           C
ATOM   339  CB  GLU A  62      21.559  22.852  43.183  1.00 41.20           C
ATOM   340  CG  GLU A  62      22.340  21.562  43.450  1.00 43.11           C
ATOM   341  CD  GLU A  62      21.455  20.385  43.790  1.00 44.30           C
ATOM   342  OE1 GLU A  62      20.626  19.994  42.931  1.00 45.50           O
ATOM   343  OE2 GLU A  62      21.590  19.850  44.917  1.00 44.82           O
ATOM   344  C   GLU A  62      23.026  24.374  44.487  1.00 39.48           C
ATOM   345  O   GLU A  62      22.459  25.187  45.226  1.00 40.03           O
ATOM   346  N   LYS A  63      24.123  23.708  44.833  1.00 38.32           N
ATOM   347  CA  LYS A  63      24.772  23.827  46.135  1.00 37.54           C
ATOM   348  CB  LYS A  63      26.033  22.956  46.148  1.00 36.71           C
ATOM   349  CG  LYS A  63      25.795  21.494  45.761  1.00 36.22           C
ATOM   350  CD  LYS A  63      24.954  20.758  46.796  1.00 35.50           C
ATOM   351  CE  LYS A  63      24.888  19.257  46.509  1.00 34.57           C
ATOM   352  NZ  LYS A  63      24.287  18.933  45.180  1.00 33.47           N
ATOM   353  C   LYS A  63      25.130  25.233  46.623  1.00 37.13           C
ATOM   354  O   LYS A  63      25.354  26.153  45.833  1.00 37.17           O
ATOM   355  N   SER A  64      25.180  25.376  47.944  1.00 36.87           N
ATOM   356  CA  SER A  64      25.531  26.637  48.590  1.00 36.73           C
ATOM   357  CB  SER A  64      25.270  26.553  50.096  1.00 36.69           C
ATOM   358  OG  SER A  64      23.936  26.162  50.370  1.00 37.39           O
ATOM   359  C   SER A  64      27.017  26.869  48.360  1.00 36.81           C
ATOM   360  O   SER A  64      27.801  25.915  48.358  1.00 36.64           O
ATOM   361  N   GLU A  65      27.410  28.125  48.177  1.00 36.66           N
ATOM   362  CA  GLU A  65      28.813  28.439  47.947  1.00 36.97           C
```

Figure 10H

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ATOM  363  CB  GLU A  65      28.985  29.926  47.611  1.00 38.23           C
ATOM  364  CG  GLU A  65      28.742  30.243  46.138  1.00 40.25           C
ATOM  365  CD  GLU A  65      28.841  31.730  45.815  1.00 42.02           C
ATOM  366  OE1 GLU A  65      29.763  32.403  46.336  1.00 43.02           O
ATOM  367  OE2 GLU A  65      28.006  32.223  45.023  1.00 43.06           O
ATOM  368  C   GLU A  65      29.702  28.050  49.122  1.00 36.16           C
ATOM  369  O   GLU A  65      30.831  27.606  48.917  1.00 36.24           O
ATOM  370  N   ALA A  66      29.198  28.202  50.345  1.00 35.06           N
ATOM  371  CA  ALA A  66      29.972  27.845  51.536  1.00 34.39           C
ATOM  372  CB  ALA A  66      29.191  28.190  52.794  1.00 34.26           C
ATOM  373  C   ALA A  66      30.317  26.348  51.522  1.00 33.80           C
ATOM  374  O   ALA A  66      31.420  25.943  51.903  1.00 33.49           O
ATOM  375  N   PHE A  67      29.367  25.528  51.087  1.00 32.84           N
ATOM  376  CA  PHE A  67      29.598  24.091  51.009  1.00 31.99           C
ATOM  377  CB  PHE A  67      28.308  23.339  50.657  1.00 31.83           C
ATOM  378  CG  PHE A  67      28.550  21.930  50.191  1.00 31.22           C
ATOM  379  CD1 PHE A  67      28.891  20.928  51.098  1.00 31.15           C
ATOM  380  CD2 PHE A  67      28.526  21.625  48.834  1.00 31.38           C
ATOM  381  CE1 PHE A  67      29.211  19.639  50.657  1.00 30.97           C
ATOM  382  CE2 PHE A  67      28.846  20.337  48.384  1.00 31.33           C
ATOM  383  CZ  PHE A  67      29.189  19.346  49.301  1.00 30.62           C
ATOM  384  C   PHE A  67      30.643  23.796  49.936  1.00 31.40           C
ATOM  385  O   PHE A  67      31.613  23.082  50.186  1.00 31.16           O
ATOM  386  N   ILE A  68      30.433  24.350  48.744  1.00 30.67           N
ATOM  387  CA  ILE A  68      31.338  24.139  47.618  1.00 30.11           C
ATOM  388  CB  ILE A  68      30.926  25.003  46.394  1.00 29.93           C
ATOM  389  CG2 ILE A  68      31.983  24.902  45.294  1.00 29.25           C
ATOM  390  CG1 ILE A  68      29.568  24.533  45.858  1.00 30.20           C
ATOM  391  CD1 ILE A  68      29.116  25.245  44.591  1.00 30.32           C
ATOM  392  C   ILE A  68      32.809  24.414  47.944  1.00 30.38           C
ATOM  393  O   ILE A  68      33.679  23.591  47.649  1.00 29.53           O
ATOM  394  N   VAL A  69      33.092  25.567  48.545  1.00 30.39           N
ATOM  395  CA  VAL A  69      34.470  25.907  48.886  1.00 30.68           C
ATOM  396  CB  VAL A  69      34.557  27.290  49.579  1.00 31.33           C
ATOM  397  CG1 VAL A  69      35.998  27.578  49.994  1.00 31.13           C
ATOM  398  CG2 VAL A  69      34.052  28.376  48.631  1.00 31.78           C
ATOM  399  C   VAL A  69      35.085  24.851  49.801  1.00 30.46           C
ATOM  400  O   VAL A  69      36.175  24.349  49.523  1.00 30.83           O
ATOM  401  N   GLU A  70      34.379  24.508  50.878  1.00 29.88           N
ATOM  402  CA  GLU A  70      34.869  23.518  51.834  1.00 30.07           C
ATOM  403  CB  GLU A  70      33.899  23.369  53.016  1.00 31.73           C
ATOM  404  CG  GLU A  70      33.763  24.597  53.925  1.00 35.37           C
ATOM  405  CD  GLU A  70      35.085  25.046  54.534  1.00 37.49           C
ATOM  406  OE1 GLU A  70      35.894  24.179  54.938  1.00 39.42           O
ATOM  407  OE2 GLU A  70      35.314  26.273  54.619  1.00 39.33           O
ATOM  408  C   GLU A  70      35.064  22.148  51.191  1.00 28.57           C
ATOM  409  O   GLU A  70      36.051  21.452  51.458  1.00 28.03           O
ATOM  410  N   ARG A  71      34.109  21.768  50.354  1.00 26.83           N
ATOM  411  CA  ARG A  71      34.140  20.478  49.677  1.00 25.52           C
ATOM  412  CB  ARG A  71      32.827  20.259  48.919  1.00 25.00           C
ATOM  413  CG  ARG A  71      32.717  18.924  48.195  1.00 24.55           C
ATOM  414  CD  ARG A  71      32.741  17.739  49.156  1.00 24.30           C
ATOM  415  NE  ARG A  71      32.481  16.490  48.437  1.00 24.43           N
ATOM  416  CZ  ARG A  71      32.569  15.278  48.973  1.00 24.76           C
ATOM  417  NH1 ARG A  71      32.915  15.130  50.248  1.00 24.34           N
ATOM  418  NH2 ARG A  71      32.321  14.210  48.227  1.00 24.54           N
ATOM  419  C   ARG A  71      35.320  20.345  48.722  1.00 24.66           C
ATOM  420  O   ARG A  71      36.044  19.352  48.769  1.00 24.09           O
```

Figure 10I

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ATOM   421  N  VAL A  72     35.521  21.342  47.863  1.00 23.70      N
ATOM   422  CA VAL A  72     36.622  21.279  46.909  1.00 23.69      C
ATOM   423  CB VAL A  72     36.537  22.428  45.883  1.00 23.55      C
ATOM   424  CG1 VAL A  72     37.697  22.337  44.904  1.00 23.48      C
ATOM   425  CG2 VAL A  72     35.206  22.337  45.125  1.00 24.07      C
ATOM   426  C  VAL A  72     37.976  21.301  47.623  1.00 23.44      C
ATOM   427  O  VAL A  72     38.907  20.607  47.216  1.00 23.28      O
ATOM   428  N  VAL A  73     38.085  22.088  48.686  1.00 23.43      N
ATOM   429  CA VAL A  73     39.326  22.139  49.451  1.00 23.42      C
ATOM   430  CB VAL A  73     39.264  23.209  50.571  1.00 24.16      C
ATOM   431  CG1 VAL A  73     40.438  23.033  51.540  1.00 24.47      C
ATOM   432  CG2 VAL A  73     39.316  24.604  49.964  1.00 24.03      C
ATOM   433  C  VAL A  73     39.578  20.755  50.076  1.00 23.35      C
ATOM   434  O  VAL A  73     40.707  20.277  50.094  1.00 23.23      O
ATOM   435  N  ALA A  74     38.527  20.108  50.575  1.00 22.61      N
ATOM   436  CA ALA A  74     38.679  18.782  51.179  1.00 22.36      C
ATOM   437  CB ALA A  74     37.382  18.355  51.870  1.00 22.18      C
ATOM   438  C  ALA A  74     39.085  17.736  50.132  1.00 22.47      C
ATOM   439  O  ALA A  74     39.916  16.867  50.400  1.00 21.70      O
ATOM   440  N  ILE A  75     38.499  17.806  48.940  1.00 22.12      N
ATOM   441  CA ILE A  75     38.857  16.845  47.911  1.00 22.33      C
ATOM   442  CB ILE A  75     37.898  16.942  46.695  1.00 22.09      C
ATOM   443  CG2 ILE A  75     38.439  16.106  45.531  1.00 21.64      C
ATOM   444  CG1 ILE A  75     36.502  16.455  47.107  1.00 22.35      C
ATOM   445  CD1 ILE A  75     35.414  16.664  46.055  1.00 21.88      C
ATOM   446  C  ILE A  75     40.319  17.017  47.460  1.00 22.41      C
ATOM   447  O  ILE A  75     41.038  16.033  47.306  1.00 22.76      O
ATOM   448  N  VAL A  76     40.770  18.253  47.259  1.00 22.98      N
ATOM   449  CA VAL A  76     42.157  18.464  46.831  1.00 22.84      C
ATOM   450  CB VAL A  76     42.436  19.945  46.478  1.00 23.18      C
ATOM   451  CG1 VAL A  76     43.922  20.122  46.125  1.00 23.17      C
ATOM   452  CG2 VAL A  76     41.557  20.376  45.294  1.00 22.52      C
ATOM   453  C  VAL A  76     43.106  18.030  47.951  1.00 23.01      C
ATOM   454  O  VAL A  76     44.206  17.542  47.706  1.00 22.66      O
ATOM   455  N  THR A  77     42.672  18.207  49.190  1.00 23.25      N
ATOM   456  CA THR A  77     43.482  17.802  50.329  1.00 23.42      C
ATOM   457  CB THR A  77     42.804  18.220  51.640  1.00 23.36      C
ATOM   458  OG1 THR A  77     42.715  19.650  51.672  1.00 23.52      O
ATOM   459  CG2 THR A  77     43.604  17.737  52.851  1.00 23.84      C
ATOM   460  C  THR A  77     43.673  16.285  50.305  1.00 23.65      C
ATOM   461  O  THR A  77     44.781  15.784  50.526  1.00 23.58      O
ATOM   462  N  ALA A  78     42.592  15.562  50.024  1.00 23.68      N
ATOM   463  CA ALA A  78     42.635  14.104  49.973  1.00 24.18      C
ATOM   464  CB ALA A  78     41.222  13.534  49.835  1.00 24.04      C
ATOM   465  C  ALA A  78     43.505  13.632  48.817  1.00 24.10      C
ATOM   466  O  ALA A  78     44.275  12.683  48.960  1.00 23.96      O
ATOM   467  N  VAL A  79     43.389  14.288  47.667  1.00 23.77      N
ATOM   468  CA VAL A  79     44.206  13.892  46.533  1.00 24.22      C
ATOM   469  CB VAL A  79     43.880  14.714  45.264  1.00 23.88      C
ATOM   470  CG1 VAL A  79     44.830  14.320  44.145  1.00 23.31      C
ATOM   471  CG2 VAL A  79     42.434  14.466  44.834  1.00 23.95      C
ATOM   472  C  VAL A  79     45.683  14.086  46.874  1.00 24.69      C
ATOM   473  O  VAL A  79     46.505  13.204  46.612  1.00 24.55      O
ATOM   474  N  GLN A  80     46.005  15.234  47.465  1.00 25.87      N
ATOM   475  CA GLN A  80     47.381  15.560  47.847  1.00 27.88      C
ATOM   476  CB GLN A  80     47.449  16.934  48.524  1.00 28.24      C
ATOM   477  CG GLN A  80     48.853  17.292  49.006  1.00 29.92      C
ATOM   478  CD GLN A  80     48.950  18.668  49.616  1.00 30.55      C
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Figure 10J

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ATOM   479 OE1 GLN A 80     48.356 18.943 50.662 1.00 32.95      O
ATOM   480 NE2 GLN A 80     49.703 19.546 48.971 1.00 31.00      N
ATOM   481 C   GLN A 80     47.991 14.521 48.781 1.00 29.34      C
ATOM   482 O   GLN A 80     49.211 14.361 48.833 1.00 28.95      O
ATOM   483 N   GLU A 81     47.143 13.824 49.527 1.00 30.79      N
ATOM   484 CA  GLU A 81     47.617 12.799 50.445 1.00 32.53      C
ATOM   485 CB  GLU A 81     46.525 12.443 51.453 1.00 34.55      C
ATOM   486 CG  GLU A 81     46.442 13.408 52.606 1.00 37.85      C
ATOM   487 CD  GLU A 81     47.735 13.457 53.399 1.00 39.61      C
ATOM   488 OE1 GLU A 81     48.230 12.381 53.806 1.00 41.29      O
ATOM   489 OE2 GLU A 81     48.258 14.569 53.618 1.00 41.33      O
ATOM   490 C   GLU A 81     48.035 11.559 49.675 1.00 32.42      C
ATOM   491 O   GLU A 81     48.974 10.865 50.066 1.00 32.74      O
ATOM   492 N   ARG A 82     47.337 11.285 48.578 1.00 31.81      N
ATOM   493 CA  ARG A 82     47.653 10.135 47.743 1.00 31.83      C
ATOM   494 CB  ARG A 82     46.456  9.777 46.852 1.00 32.76      C
ATOM   495 CG  ARG A 82     45.289  9.128 47.600 1.00 34.95      C
ATOM   496 CD  ARG A 82     45.701  7.773 48.180 1.00 36.27      C
ATOM   497 NE  ARG A 82     45.997  6.810 47.120 1.00 38.20      N
ATOM   498 CZ  ARG A 82     45.085  6.042 46.528 1.00 38.36      C
ATOM   499 NH1 ARG A 82     43.815  6.116 46.899 1.00 38.95      N
ATOM   500 NH2 ARG A 82     45.441  5.212 45.554 1.00 38.87      N
ATOM   501 C   ARG A 82     48.879 10.431 46.877 1.00 31.32      C
ATOM   502 O   ARG A 82     49.741  9.568 46.690 1.00 31.21      O
ATOM   503 N   TYR A 83     48.953 11.650 46.351 1.00 30.58      N
ATOM   504 CA  TYR A 83     50.079 12.057 45.510 1.00 30.30      C
ATOM   505 CB  TYR A 83     49.798 11.802 44.021 1.00 30.71      C
ATOM   506 CG  TYR A 83     49.710 10.362 43.580 1.00 31.39      C
ATOM   507 CD1 TYR A 83     48.481  9.717 43.484 1.00 31.23      C
ATOM   508 CE1 TYR A 83     48.394  8.404 43.034 1.00 32.06      C
ATOM   509 CD2 TYR A 83     50.857  9.655 43.218 1.00 31.62      C
ATOM   510 CE2 TYR A 83     50.780  8.342 42.767 1.00 32.08      C
ATOM   511 CZ  TYR A 83     49.550  7.724 42.677 1.00 32.19      C
ATOM   512 OH  TYR A 83     49.471  6.423 42.229 1.00 32.58      O
ATOM   513 C   TYR A 83     50.408 13.538 45.629 1.00 29.65      C
ATOM   514 O   TYR A 83     49.520 14.385 45.519 1.00 29.22      O
ATOM   515 N   PRO A 84     51.685 13.872 45.875 1.00 29.11      N
ATOM   516 CD  PRO A 84     52.799 13.019 46.335 1.00 29.50      C
ATOM   517 CA  PRO A 84     52.034 15.291 45.966 1.00 28.54      C
ATOM   518 CB  PRO A 84     53.539 15.257 46.206 1.00 29.05      C
ATOM   519 CG  PRO A 84     53.700 14.012 47.048 1.00 29.74      C
ATOM   520 C   PRO A 84     51.681 15.839 44.579 1.00 27.78      C
ATOM   521 O   PRO A 84     51.882 15.156 43.576 1.00 27.15      O
ATOM   522 N   LEU A 85     51.151 17.053 44.518 1.00 27.35      N
ATOM   523 CA  LEU A 85     50.741 17.626 43.239 1.00 26.90      C
ATOM   524 CB  LEU A 85     49.323 18.192 43.361 1.00 26.62      C
ATOM   525 CG  LEU A 85     48.230 17.259 43.889 1.00 26.34      C
ATOM   526 CD1 LEU A 85     46.923 18.030 44.073 1.00 26.18      C
ATOM   527 CD2 LEU A 85     48.049 16.102 42.926 1.00 26.09      C
ATOM   528 C   LEU A 85     51.661 18.725 42.731 1.00 26.93      C
ATOM   529 O   LEU A 85     52.148 19.540 43.501 1.00 26.47      O
ATOM   530 N   ALA A 86     51.908 18.731 41.428 1.00 27.16      N
ATOM   531 CA  ALA A 86     52.727 19.772 40.828 1.00 27.51      C
ATOM   532 CB  ALA A 86     53.411 19.244 39.560 1.00 27.79      C
ATOM   533 C   ALA A 86     51.775 20.922 40.484 1.00 27.57      C
ATOM   534 O   ALA A 86     52.149 22.091 40.512 1.00 28.41      O
ATOM   535 N   LEU A 87     50.524 20.581 40.189 1.00 27.71      N
ATOM   536 CA  LEU A 87     49.530 21.582 39.824 1.00 27.37      C
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Figure 10K

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ATOM   537 CB  LEU A  87    49.866  22.133  38.430  1.00 28.02      C
ATOM   538 CG  LEU A  87    48.916  23.067  37.676  1.00 27.98      C
ATOM   539 CD1 LEU A  87    49.721  23.825  36.624  1.00 28.10      C
ATOM   540 CD2 LEU A  87    47.788  22.274  37.013  1.00 28.31      C
ATOM   541 C   LEU A  87    48.134  20.972  39.817  1.00 27.07      C
ATOM   542 O   LEU A  87    47.973  19.779  39.558  1.00 27.09      O
ATOM   543 N   ALA A  88    47.132  21.797  40.101  1.00 26.70      N
ATOM   544 CA  ALA A  88    45.745  21.353  40.106  1.00 26.24      C
ATOM   545 CB  ALA A  88    45.218  21.285  41.528  1.00 26.54      C
ATOM   546 C   ALA A  88    44.876  22.299  39.282  1.00 26.33      C
ATOM   547 O   ALA A  88    45.040  23.522  39.326  1.00 25.93      O
ATOM   548 N   VAL A  89    43.949  21.719  38.532  1.00 26.38      N
ATOM   549 CA  VAL A  89    43.035  22.493  37.704  1.00 26.48      C
ATOM   550 CB  VAL A  89    43.100  22.057  36.225  1.00 26.98      C
ATOM   551 CG1 VAL A  89    42.184  22.945  35.388  1.00 26.51      C
ATOM   552 CG2 VAL A  89    44.535  22.111  35.719  1.00 26.37      C
ATOM   553 C   VAL A  89    41.605  22.285  38.174  1.00 26.45      C
ATOM   554 O   VAL A  89    41.128  21.153  38.248  1.00 26.61      O
ATOM   555 N   VAL A  90    40.930  23.375  38.513  1.00 26.03      N
ATOM   556 CA  VAL A  90    39.543  23.300  38.928  1.00 26.42      C
ATOM   557 CB  VAL A  90    39.195  24.432  39.916  1.00 26.37      C
ATOM   558 CG1 VAL A  90    37.744  24.315  40.361  1.00 26.82      C
ATOM   559 CG2 VAL A  90    40.123  24.355  41.137  1.00 26.76      C
ATOM   560 C   VAL A  90    38.787  23.490  37.615  1.00 26.74      C
ATOM   561 O   VAL A  90    38.371  24.601  37.288  1.00 26.48      O
ATOM   562 N   ALA A  91    38.657  22.405  36.853  1.00 26.82      N
ATOM   563 CA  ALA A  91    37.986  22.438  35.549  1.00 27.63      C
ATOM   564 CB  ALA A  91    38.468  21.276  34.694  1.00 27.04      C
ATOM   565 C   ALA A  91    36.488  22.356  35.758  1.00 28.11      C
ATOM   566 O   ALA A  91    35.820  21.459  35.242  1.00 27.96      O
ATOM   567 N   CYS A  92    35.979  23.327  36.509  1.00 29.18      N
ATOM   568 CA  CYS A  92    34.579  23.399  36.882  1.00 30.48      C
ATOM   569 CB  CYS A  92    34.402  22.573  38.163  1.00 30.27      C
ATOM   570 SG  CYS A  92    32.819  22.659  38.984  1.00 30.88      S
ATOM   571 C   CYS A  92    34.219  24.867  37.137  1.00 31.39      C
ATOM   572 O   CYS A  92    34.730  25.473  38.075  1.00 31.00      O
ATOM   573 N   ASN A  93    33.341  25.436  36.310  1.00 32.97      N
ATOM   574 CA  ASN A  93    32.937  26.837  36.470  1.00 34.50      C
ATOM   575 CB  ASN A  93    32.043  27.283  35.306  1.00 35.30      C
ATOM   576 CG  ASN A  93    32.770  27.298  33.982  1.00 36.40      C
ATOM   577 OD1 ASN A  93    32.983  26.251  33.360  1.00 37.59      O
ATOM   578 ND2 ASN A  93    33.165  28.489  33.539  1.00 36.95      N
ATOM   579 C   ASN A  93    32.218  27.128  37.784  1.00 35.02      C
ATOM   580 O   ASN A  93    32.473  28.151  38.426  1.00 35.62      O
ATOM   581 N   THR A  94    31.317  26.236  38.183  1.00 35.16      N
ATOM   582 CA  THR A  94    30.567  26.418  39.420  1.00 36.16      C
ATOM   583 CB  THR A  94    29.417  25.389  39.539  1.00 36.42      C
ATOM   584 OG1 THR A  94    29.934  24.063  39.353  1.00 36.99      O
ATOM   585 CG2 THR A  94    28.354  25.662  38.493  1.00 36.28      C
ATOM   586 C   THR A  94    31.436  26.311  40.668  1.00 36.39      C
ATOM   587 O   THR A  94    30.972  26.572  41.774  1.00 37.04      O
ATOM   588 N   ALA A  95    32.695  25.928  40.501  1.00 36.62      N
ATOM   589 CA  ALA A  95    33.587  25.803  41.654  1.00 37.07      C
ATOM   590 CB  ALA A  95    34.093  24.363  41.780  1.00 36.87      C
ATOM   591 C   ALA A  95    34.769  26.757  41.599  1.00 37.26      C
ATOM   592 O   ALA A  95    35.183  27.291  42.626  1.00 37.43      O
ATOM   593 N   SER A  96    35.304  26.978  40.405  1.00 37.85      N
ATOM   594 CA  SER A  96    36.464  27.844  40.245  1.00 38.98      C
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Figure 10L

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ATOM   595 CB  SER A  96    36.701  28.167  38.772  1.00 38.43      C
ATOM   596 OG  SER A  96    37.534  27.193  38.172  1.00 39.50      O
ATOM   597 C   SER A  96    36.403  29.140  41.031  1.00 39.55      C
ATOM   598 O   SER A  96    37.056  29.276  42.064  1.00 40.03      O
ATOM   599 N   THR A  97    35.621  30.090  40.540  1.00 40.03      N
ATOM   600 CA  THR A  97    35.507  31.386  41.193  1.00 40.80      C
ATOM   601 CB  THR A  97    34.206  32.086  40.782  1.00 41.54      C
ATOM   602 OG1 THR A  97    33.079  31.351  41.283  1.00 43.65      O
ATOM   603 CG2 THR A  97    34.116  32.152  39.266  1.00 42.47      C
ATOM   604 C   THR A  97    35.580  31.334  42.718  1.00 40.13      C
ATOM   605 O   THR A  97    36.587  31.730  43.322  1.00 40.25      O
ATOM   606 N   VAL A  98    34.524  30.819  43.333  1.00 38.98      N
ATOM   607 CA  VAL A  98    34.440  30.749  44.783  1.00 37.63      C
ATOM   608 CB  VAL A  98    33.074  30.183  45.210  1.00 38.05      C
ATOM   609 CG1 VAL A  98    31.951  31.032  44.616  1.00 37.94      C
ATOM   610 CG2 VAL A  98    32.949  28.735  44.752  1.00 37.58      C
ATOM   611 C   VAL A  98    35.521  29.956  45.520  1.00 36.84      C
ATOM   612 O   VAL A  98    35.789  30.230  46.689  1.00 36.41      O
ATOM   613 N   SER A  99    36.145  28.989  44.848  1.00 35.65      N
ATOM   614 CA  SER A  99    37.149  28.136  45.491  1.00 34.62      C
ATOM   615 CB  SER A  99    36.982  26.688  45.001  1.00 34.67      C
ATOM   616 OG  SER A  99    35.697  26.177  45.311  1.00 35.45      O
ATOM   617 C   SER A  99    38.626  28.504  45.353  1.00 33.65      C
ATOM   618 O   SER A  99    39.443  28.075  46.165  1.00 33.61      O
ATOM   619 N   LEU A 100    38.974  29.278  44.335  1.00 32.41      N
ATOM   620 CA  LEU A 100    40.371  29.635  44.103  1.00 31.86      C
ATOM   621 CB  LEU A 100    40.476  30.501  42.844  1.00 31.39      C
ATOM   622 CG  LEU A 100    40.052  29.816  41.538  1.00 31.77      C
ATOM   623 CD1 LEU A 100    40.345  30.741  40.359  1.00 31.20      C
ATOM   624 CD2 LEU A 100    40.813  28.498  41.363  1.00 31.65      C
ATOM   625 C   LEU A 100    41.131  30.286  45.272  1.00 31.53      C
ATOM   626 O   LEU A 100    42.227  29.851  45.620  1.00 31.21      O
ATOM   627 N   PRO A 101    40.570  31.336  45.887  1.00 31.41      N
ATOM   628 CD  PRO A 101    39.378  32.122  45.526  1.00 31.74      C
ATOM   629 CA  PRO A 101    41.289  31.958  47.006  1.00 31.39      C
ATOM   630 CB  PRO A 101    40.312  33.027  47.488  1.00 31.54      C
ATOM   631 CG  PRO A 101    39.657  33.455  46.202  1.00 31.94      C
ATOM   632 C   PRO A 101    41.642  30.960  48.111  1.00 31.01      C
ATOM   633 O   PRO A 101    42.784  30.908  48.574  1.00 30.97      O
ATOM   634 N   ALA A 102    40.657  30.168  48.522  1.00 30.66      N
ATOM   635 CA  ALA A 102    40.845  29.180  49.579  1.00 30.28      C
ATOM   636 CB  ALA A 102    39.507  28.531  49.927  1.00 30.65      C
ATOM   637 C   ALA A 102    41.867  28.110  49.210  1.00 29.99      C
ATOM   638 O   ALA A 102    42.675  27.692  50.049  1.00 29.77      O
ATOM   639 N   LEU A 103    41.833  27.668  47.957  1.00 29.36      N
ATOM   640 CA  LEU A 103    42.764  26.650  47.483  1.00 28.42      C
ATOM   641 CB  LEU A 103    42.322  26.126  46.119  1.00 27.97      C
ATOM   642 CG  LEU A 103    41.031  25.302  46.119  1.00 27.49      C
ATOM   643 CD1 LEU A 103    40.535  25.118  44.684  1.00 26.76      C
ATOM   644 CD2 LEU A 103    41.286  23.957  46.790  1.00 26.64      C
ATOM   645 C   LEU A 103    44.184  27.189  47.378  1.00 28.66      C
ATOM   646 O   LEU A 103    45.145  26.503  47.722  1.00 27.90      O
ATOM   647 N   ARG A 104    44.315  28.424  46.911  1.00 28.64      N
ATOM   648 CA  ARG A 104    45.630  29.021  46.761  1.00 29.38      C
ATOM   649 CB  ARG A 104    45.540  30.265  45.875  1.00 29.44      C
ATOM   650 CG  ARG A 104    45.362  29.904  44.407  1.00 30.55      C
ATOM   651 CD  ARG A 104    44.967  31.091  43.526  1.00 31.09      C
ATOM   652 NE  ARG A 104    44.866  30.655  42.134  1.00 31.83      N
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Figure 10M

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ATOM   653  CZ  ARG A 104      44.212  31.307  41.175  1.00 31.39      C
ATOM   654  NH1 ARG A 104      43.585  32.442  41.439  1.00 31.47      N
ATOM   655  NH2 ARG A 104      44.180  30.810  39.950  1.00 30.99      N
ATOM   656  C   ARG A 104      46.261  29.346  48.104  1.00 29.24      C
ATOM   657  O   ARG A 104      47.477  29.439  48.213  1.00 28.87      O
ATOM   658  N   GLU A 105      45.430  29.507  49.126  1.00 29.80      N
ATOM   659  CA  GLU A 105      45.928  29.791  50.465  1.00 31.03      C
ATOM   660  CB  GLU A 105      44.831  30.424  51.328  1.00 32.41      C
ATOM   661  CG  GLU A 105      45.138  30.405  52.827  1.00 34.95      C
ATOM   662  CD  GLU A 105      46.373  31.213  53.190  1.00 36.39      C
ATOM   663  OE1 GLU A 105      46.929  30.992  54.294  1.00 37.63      O
ATOM   664  OE2 GLU A 105      46.785  32.072  52.379  1.00 37.49      O
ATOM   665  C   GLU A 105      46.408  28.503  51.129  1.00 30.44      C
ATOM   666  O   GLU A 105      47.463  28.476  51.761  1.00 31.06      O
ATOM   667  N   LYS A 106      45.648  27.428  50.972  1.00 29.73      N
ATOM   668  CA  LYS A 106      46.023  26.175  51.605  1.00 29.26      C
ATOM   669  CB  LYS A 106      44.806  25.245  51.723  1.00 29.20      C
ATOM   670  CG  LYS A 106      45.091  24.005  52.595  1.00 29.25      C
ATOM   671  CD  LYS A 106      43.840  23.174  52.882  1.00 28.92      C
ATOM   672  CE  LYS A 106      44.150  22.010  53.840  1.00 28.67      C
ATOM   673  NZ  LYS A 106      42.965  21.124  54.082  1.00 28.66      N
ATOM   674  C   LYS A 106      47.168  25.410  50.943  1.00 29.05      C
ATOM   675  O   LYS A 106      47.993  24.806  51.635  1.00 28.51      O
ATOM   676  N   PHE A 107      47.240  25.445  49.617  1.00 28.37      N
ATOM   677  CA  PHE A 107      48.270  24.690  48.925  1.00 28.51      C
ATOM   678  CB  PHE A 107      47.627  23.857  47.815  1.00 28.11      C
ATOM   679  CG  PHE A 107      46.516  22.973  48.308  1.00 27.86      C
ATOM   680  CD1 PHE A 107      45.185  23.346  48.147  1.00 27.53      C
ATOM   681  CD2 PHE A 107      46.805  21.795  48.991  1.00 27.75      C
ATOM   682  CE1 PHE A 107      44.156  22.560  48.665  1.00 27.08      C
ATOM   683  CE2 PHE A 107      45.781  20.997  49.514  1.00 27.41      C
ATOM   684  CZ  PHE A 107      44.457  21.383  49.350  1.00 27.01      C
ATOM   685  C   PHE A 107      49.443  25.476  48.376  1.00 28.85      C
ATOM   686  O   PHE A 107      49.337  26.669  48.096  1.00 28.61      O
ATOM   687  N   ASP A 108      50.566  24.781  48.225  1.00 29.16      N
ATOM   688  CA  ASP A 108      51.781  25.394  47.716  1.00 29.72      C
ATOM   689  CB  ASP A 108      52.925  25.180  48.700  1.00 29.47      C
ATOM   690  CG  ASP A 108      52.721  25.959  49.973  1.00 29.74      C
ATOM   691  OD1 ASP A 108      52.567  27.196  49.880  1.00 29.19      O
ATOM   692  OD2 ASP A 108      52.700  25.344  51.058  1.00 29.72      O
ATOM   693  C   ASP A 108      52.163  24.914  46.333  1.00 29.83      C
ATOM   694  O   ASP A 108      53.335  24.699  46.018  1.00 30.36      O
ATOM   695  N   PHE A 109      51.145  24.724  45.511  1.00 29.48      N
ATOM   696  CA  PHE A 109      51.345  24.342  44.128  1.00 29.36      C
ATOM   697  CB  PHE A 109      51.079  22.844  43.895  1.00 28.81      C
ATOM   698  CG  PHE A 109      49.781  22.348  44.454  1.00 29.18      C
ATOM   699  CD1 PHE A 109      48.568  22.679  43.851  1.00 29.09      C
ATOM   700  CD2 PHE A 109      49.772  21.525  45.579  1.00 28.19      C
ATOM   701  CE1 PHE A 109      47.363  22.194  44.364  1.00 29.20      C
ATOM   702  CE2 PHE A 109      48.580  21.037  46.099  1.00 28.87      C
ATOM   703  CZ  PHE A 109      47.368  21.369  45.492  1.00 28.19      C
ATOM   704  C   PHE A 109      50.358  25.232  43.397  1.00 28.99      C
ATOM   705  O   PHE A 109      49.331  25.626  43.956  1.00 28.79      O
ATOM   706  N   PRO A 110      50.673  25.600  42.153  1.00 29.04      N
ATOM   707  CD  PRO A 110      51.823  25.213  41.318  1.00 28.89      C
ATOM   708  CA  PRO A 110      49.751  26.467  41.419  1.00 29.02      C
ATOM   709  CB  PRO A 110      50.515  26.761  40.128  1.00 28.79      C
ATOM   710  CG  PRO A 110      51.326  25.525  39.929  1.00 29.59      C
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Figure 10N

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ATOM   711  C  PRO A 110    48.381  25.839  41.182  1.00 28.61      C
ATOM   712  O  PRO A 110    48.259  24.630  40.990  1.00 28.77      O
ATOM   713  N  VAL A 111    47.352  26.673  41.224  1.00 28.61      N
ATOM   714  CA VAL A 111    45.989  26.215  41.002  1.00 28.17      C
ATOM   715  CB VAL A 111    45.101  26.457  42.240  1.00 27.94      C
ATOM   716  CG1 VAL A 111    43.683  25.945  41.978  1.00 26.91      C
ATOM   717  CG2 VAL A 111    45.710  25.759  43.467  1.00 27.23      C
ATOM   718  C  VAL A 111    45.417  26.987  39.822  1.00 28.51      C
ATOM   719  O  VAL A 111    45.482  28.213  39.786  1.00 28.55      O
ATOM   720  N  VAL A 112    44.871  26.263  38.854  1.00 28.78      N
ATOM   721  CA VAL A 112    44.284  26.892  37.679  1.00 29.08      C
ATOM   722  CB VAL A 112    44.691  26.145  36.387  1.00 29.31      C
ATOM   723  CG1 VAL A 112    43.996  26.753  35.175  1.00 29.34      C
ATOM   724  CG2 VAL A 112    46.185  26.215  36.213  1.00 28.86      C
ATOM   725  C  VAL A 112    42.772  26.891  37.810  1.00 29.49      C
ATOM   726  O  VAL A 112    42.175  25.895  38.227  1.00 29.47      O
ATOM   727  N  GLY A 113    42.160  28.021  37.475  1.00 29.33      N
ATOM   728  CA GLY A 113    40.719  28.132  37.551  1.00 29.94      C
ATOM   729  C  GLY A 113    40.136  28.309  36.164  1.00 30.66      C
ATOM   730  O  GLY A 113    40.873  28.407  35.180  1.00 29.81      O
ATOM   731  N  VAL A 114    38.809  28.351  36.088  1.00 31.45      N
ATOM   732  CA VAL A 114    38.121  28.518  34.811  1.00 32.36      C
ATOM   733  CB VAL A 114    37.509  27.204  34.315  1.00 32.77      C
ATOM   734  CG1 VAL A 114    38.587  26.138  34.165  1.00 32.86      C
ATOM   735  CG2 VAL A 114    36.425  26.756  35.276  1.00 33.24      C
ATOM   736  C  VAL A 114    36.983  29.521  34.894  1.00 32.64      C
ATOM   737  O  VAL A 114    36.178  29.505  35.833  1.00 33.94      O
ATOM   738  N  VAL A 115    36.932  30.409  33.913  1.00 31.91      N
ATOM   739  CA VAL A 115    35.869  31.395  33.830  1.00 31.47      C
ATOM   740  CB VAL A 115    36.368  32.820  34.173  1.00 32.15      C
ATOM   741  CG1 VAL A 115    36.717  32.908  35.652  1.00 33.28      C
ATOM   742  CG2 VAL A 115    37.579  33.169  33.330  1.00 32.44      C
ATOM   743  C  VAL A 115    35.409  31.348  32.375  1.00 30.19      C
ATOM   744  O  VAL A 115    36.202  31.048  31.483  1.00 29.34      O
ATOM   745  N  PRO A 116    34.122  31.615  32.121  1.00 29.68      N
ATOM   746  CD PRO A 116    33.044  31.894  33.088  1.00 29.83      C
ATOM   747  CA PRO A 116    33.610  31.590  30.743  1.00 28.99      C
ATOM   748  CB PRO A 116    32.195  32.141  30.894  1.00 29.53      C
ATOM   749  CG PRO A 116    31.793  31.619  32.267  1.00 29.52      C
ATOM   750  C  PRO A 116    34.482  32.445  29.826  1.00 28.73      C
ATOM   751  O  PRO A 116    34.865  33.560  30.194  1.00 28.39      O
ATOM   752  N  ALA A 117    34.786  31.921  28.639  1.00 27.82      N
ATOM   753  CA ALA A 117    35.638  32.607  27.663  1.00 28.21      C
ATOM   754  CB ALA A 117    36.125  31.607  26.614  1.00 26.94      C
ATOM   755  C  ALA A 117    34.977  33.800  26.974  1.00 28.60      C
ATOM   756  O  ALA A 117    35.023  33.930  25.747  1.00 28.59      O
ATOM   757  N  ILE A 118    34.376  34.676  27.766  1.00 28.96      N
ATOM   758  CA ILE A 118    33.710  35.848  27.225  1.00 29.91      C
ATOM   759  CB ILE A 118    32.962  36.606  28.335  1.00 31.06      C
ATOM   760  CG2 ILE A 118    32.449  37.950  27.808  1.00 31.44      C
ATOM   761  CG1 ILE A 118    31.809  35.736  28.844  1.00 31.63      C
ATOM   762  CD1 ILE A 118    31.091  36.303  30.038  1.00 33.47      C
ATOM   763  C  ILE A 118    34.673  36.800  26.537  1.00 30.04      C
ATOM   764  O  ILE A 118    34.367  37.329  25.466  1.00 29.91      O
ATOM   765  N  LYS A 119    35.840  37.008  27.143  1.00 29.81      N
ATOM   766  CA LYS A 119    36.836  37.915  26.584  1.00 30.04      C
ATOM   767  CB LYS A 119    38.091  37.933  27.468  1.00 30.22      C
ATOM   768  CG LYS A 119    39.130  38.955  27.020  1.00 30.96      C
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Figure 10O

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ATOM   769  CD  LYS A 119      40.292  39.050  27.988  1.00 31.45           C
ATOM   770  CE  LYS A 119      41.314  40.048  27.492  1.00 31.36           C
ATOM   771  NZ  LYS A 119      42.566  39.971  28.280  1.00 32.08           N
ATOM   772  C   LYS A 119      37.210  37.606  25.125  1.00 30.26           C
ATOM   773  O   LYS A 119      37.081  38.468  24.260  1.00 30.43           O
ATOM   774  N   PRO A 120      37.687  36.385  24.829  1.00 30.32           N
ATOM   775  CD  PRO A 120      38.119  35.261  25.679  1.00 30.42           C
ATOM   776  CA  PRO A 120      38.024  36.135  23.424  1.00 30.77           C
ATOM   777  CB  PRO A 120      38.743  34.782  23.469  1.00 30.78           C
ATOM   778  CG  PRO A 120      38.175  34.123  24.687  1.00 30.65           C
ATOM   779  C   PRO A 120      36.805  36.124  22.501  1.00 31.13           C
ATOM   780  O   PRO A 120      36.900  36.515  21.339  1.00 31.33           O
ATOM   781  N   ALA A 121      35.662  35.684  23.018  1.00 31.38           N
ATOM   782  CA  ALA A 121      34.447  35.632  22.214  1.00 31.88           C
ATOM   783  CB  ALA A 121      33.317  35.001  23.007  1.00 31.22           C
ATOM   784  C   ALA A 121      34.049  37.030  21.754  1.00 32.64           C
ATOM   785  O   ALA A 121      33.558  37.206  20.637  1.00 32.09           O
ATOM   786  N   ALA A 122      34.268  38.019  22.618  1.00 33.55           N
ATOM   787  CA  ALA A 122      33.931  39.405  22.305  1.00 34.91           C
ATOM   788  CB  ALA A 122      34.108  40.281  23.544  1.00 34.63           C
ATOM   789  C   ALA A 122      34.779  39.944  21.159  1.00 35.90           C
ATOM   790  O   ALA A 122      34.334  40.809  20.408  1.00 36.06           O
ATOM   791  N   ARG A 123      36.000  39.435  21.029  1.00 37.08           N
ATOM   792  CA  ARG A 123      36.901  39.866  19.962  1.00 38.64           C
ATOM   793  CB  ARG A 123      38.363  39.696  20.382  1.00 39.68           C
ATOM   794  CG  ARG A 123      38.775  40.468  21.618  1.00 41.76           C
ATOM   795  CD  ARG A 123      40.279  40.379  21.811  1.00 43.75           C
ATOM   796  NE  ARG A 123      41.000  40.999  20.701  1.00 45.71           N
ATOM   797  CZ  ARG A 123      42.320  40.959  20.547  1.00 46.46           C
ATOM   798  NH1 ARG A 123      43.071  40.321  21.435  1.00 47.45           N
ATOM   799  NH2 ARG A 123      42.891  41.564  19.512  1.00 47.03           N
ATOM   800  C   ARG A 123      36.689  39.068  18.678  1.00 39.10           C
ATOM   801  O   ARG A 123      37.252  39.405  17.636  1.00 39.34           O
ATOM   802  N   LEU A 124      35.886  38.011  18.749  1.00 39.13           N
ATOM   803  CA  LEU A 124      35.653  37.165  17.583  1.00 39.56           C
ATOM   804  CB  LEU A 124      35.776  35.686  17.975  1.00 39.49           C
ATOM   805  CG  LEU A 124      37.133  35.224  18.517  1.00 39.90           C
ATOM   806  CD1 LEU A 124      37.039  33.765  18.952  1.00 40.24           C
ATOM   807  CD2 LEU A 124      38.210  35.398  17.455  1.00 40.03           C
ATOM   808  C   LEU A 124      34.315  37.391  16.895  1.00 39.81           C
ATOM   809  O   LEU A 124      34.197  37.192  15.685  1.00 39.83           O
ATOM   810  N   THR A 125      33.311  37.807  17.659  1.00 39.86           N
ATOM   811  CA  THR A 125      31.991  38.027  17.096  1.00 40.44           C
ATOM   812  CB  THR A 125      30.981  38.482  18.179  1.00 40.32           C
ATOM   813  OG1 THR A 125      29.685  38.636  17.589  1.00 40.44           O
ATOM   814  CG2 THR A 125      31.411  39.803  18.809  1.00 40.44           C
ATOM   815  C   THR A 125      32.023  39.057  15.971  1.00 41.06           C
ATOM   816  O   THR A 125      32.777  40.028  16.022  1.00 40.79           O
ATOM   817  N   ALA A 126      31.206  38.826  14.949  1.00 41.50           N
ATOM   818  CA  ALA A 126      31.133  39.732  13.812  1.00 42.01           C
ATOM   819  CB  ALA A 126      31.214  38.943  12.507  1.00 41.90           C
ATOM   820  C   ALA A 126      29.837  40.532  13.861  1.00 42.35           C
ATOM   821  O   ALA A 126      29.798  41.685  13.427  1.00 42.99           O
ATOM   822  N   ASN A 127      28.778  39.928  14.394  1.00 41.88           N
ATOM   823  CA  ASN A 127      27.493  40.613  14.476  1.00 41.62           C
ATOM   824  CB  ASN A 127      26.350  39.641  14.147  1.00 41.84           C
ATOM   825  CG  ASN A 127      26.027  38.692  15.291  1.00 41.92           C
ATOM   826  OD1 ASN A 127      26.847  38.451  16.175  1.00 41.99           O
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Figure 10P

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ATOM   827 ND2 ASN A 127     24.822  38.135  15.264  1.00 41.74      N
ATOM   828 C   ASN A 127     27.266  41.262  15.834  1.00 41.10      C
ATOM   829 O   ASN A 127     26.241  41.902  16.066  1.00 41.43      O
ATOM   830 N   GLY A 128     28.234  41.101  16.730  1.00 40.81      N
ATOM   831 CA  GLY A 128     28.122  41.688  18.052  1.00 39.82      C
ATOM   832 C   GLY A 128     27.185  40.965  19.004  1.00 39.18      C
ATOM   833 O   GLY A 128     26.933  41.453  20.103  1.00 39.41      O
ATOM   834 N   ILE A 129     26.660  39.812  18.594  1.00 38.60      N
ATOM   835 CA  ILE A 129     25.757  39.044  19.451  1.00 37.56      C
ATOM   836 CB  ILE A 129     24.523  38.522  18.686  1.00 37.63      C
ATOM   837 CG2 ILE A 129     23.450  38.100  19.686  1.00 37.28      C
ATOM   838 CG1 ILE A 129     23.980  39.593  17.732  1.00 38.02      C
ATOM   839 CD1 ILE A 129     23.250  40.727  18.406  1.00 38.18      C
ATOM   840 C   ILE A 129     26.510  37.822  19.983  1.00 36.88      C
ATOM   841 O   ILE A 129     26.787  36.882  19.241  1.00 36.65      O
ATOM   842 N   VAL A 130     26.834  37.840  21.270  1.00 35.90      N
ATOM   843 CA  VAL A 130     27.554  36.733  21.877  1.00 34.41      C
ATOM   844 CB  VAL A 130     28.823  37.233  22.594  1.00 34.44      C
ATOM   845 CG1 VAL A 130     29.512  36.079  23.314  1.00 34.63      C
ATOM   846 CG2 VAL A 130     29.768  37.857  21.578  1.00 33.95      C
ATOM   847 C   VAL A 130     26.674  35.990  22.870  1.00 33.52      C
ATOM   848 O   VAL A 130     26.082  36.589  23.770  1.00 33.77      O
ATOM   849 N   GLY A 131     26.583  34.679  22.695  1.00 32.38      N
ATOM   850 CA  GLY A 131     25.779  33.877  23.593  1.00 31.20      C
ATOM   851 C   GLY A 131     26.626  33.212  24.667  1.00 30.54      C
ATOM   852 O   GLY A 131     27.799  32.903  24.453  1.00 29.56      O
ATOM   853 N   LEU A 132     26.032  33.009  25.837  1.00 29.94      N
ATOM   854 CA  LEU A 132     26.726  32.348  26.930  1.00 29.63      C
ATOM   855 CB  LEU A 132     26.970  33.314  28.094  1.00 29.35      C
ATOM   856 CG  LEU A 132     27.559  32.707  29.383  1.00 29.67      C
ATOM   857 CD1 LEU A 132     28.930  32.091  29.115  1.00 28.73      C
ATOM   858 CD2 LEU A 132     27.676  33.800  30.444  1.00 29.83      C
ATOM   859 C   LEU A 132     25.870  31.189  27.402  1.00 29.56      C
ATOM   860 O   LEU A 132     24.764  31.392  27.912  1.00 29.35      O
ATOM   861 N   LEU A 133     26.362  29.975  27.190  1.00 29.49      N
ATOM   862 CA  LEU A 133     25.658  28.776  27.632  1.00 30.26      C
ATOM   863 CB  LEU A 133     25.747  27.655  26.596  1.00 29.82      C
ATOM   864 CG  LEU A 133     24.832  27.685  25.382  1.00 29.97      C
ATOM   865 CD1 LEU A 133     25.087  26.431  24.561  1.00 29.36      C
ATOM   866 CD2 LEU A 133     23.370  27.738  25.831  1.00 29.56      C
ATOM   867 C   LEU A 133     26.374  28.328  28.891  1.00 30.96      C
ATOM   868 O   LEU A 133     27.577  28.064  28.867  1.00 30.93      O
ATOM   869 N   ALA A 134     25.641  28.258  29.991  1.00 31.95      N
ATOM   870 CA  ALA A 134     26.220  27.838  31.256  1.00 33.61      C
ATOM   871 CB  ALA A 134     26.671  29.056  32.057  1.00 33.35      C
ATOM   872 C   ALA A 134     25.157  27.080  32.022  1.00 34.73      C
ATOM   873 O   ALA A 134     24.021  26.963  31.567  1.00 34.36      O
ATOM   874 N   THR A 135     25.515  26.552  33.184  1.00 36.55      N
ATOM   875 CA  THR A 135     24.522  25.845  33.960  1.00 38.50      C
ATOM   876 CB  THR A 135     25.166  24.865  34.958  1.00 38.44      C
ATOM   877 OG1 THR A 135     24.136  24.057  35.544  1.00 38.63      O
ATOM   878 CG2 THR A 135     25.932  25.610  36.037  1.00 37.99      C
ATOM   879 C   THR A 135     23.676  26.890  34.683  1.00 40.21      C
ATOM   880 O   THR A 135     24.069  28.056  34.790  1.00 39.88      O
ATOM   881 N   ARG A 136     22.514  26.470  35.169  1.00 42.42      N
ATOM   882 CA  ARG A 136     21.592  27.374  35.840  1.00 44.95      C
ATOM   883 CB  ARG A 136     20.419  26.584  36.429  1.00 44.96      C
ATOM   884 CG  ARG A 136     19.310  27.468  36.958  1.00 45.04      C
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Figure 10Q

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ATOM   885  CD  ARG A 136      18.840  28.437  35.880  1.00 44.89           C
ATOM   886  NE  ARG A 136      18.043  29.521  36.442  1.00 45.05           N
ATOM   887  CZ  ARG A 136      17.561  30.538  35.736  1.00 44.74           C
ATOM   888  NH1 ARG A 136      17.794  30.611  34.433  1.00 44.68           N
ATOM   889  NH2 ARG A 136      16.854  31.484  36.337  1.00 44.28           N
ATOM   890  C   ARG A 136      22.226  28.242  36.921  1.00 46.64           C
ATOM   891  O   ARG A 136      21.963  29.443  36.987  1.00 46.85           O
ATOM   892  N   GLY A 137      23.064  27.637  37.759  1.00 48.47           N
ATOM   893  CA  GLY A 137      23.705  28.383  38.828  1.00 50.63           C
ATOM   894  C   GLY A 137      24.761  29.390  38.405  1.00 52.15           C
ATOM   895  O   GLY A 137      24.957  30.403  39.077  1.00 52.40           O
ATOM   896  N   THR A 138      25.439  29.122  37.295  1.00 53.81           N
ATOM   897  CA  THR A 138      26.493  30.007  36.804  1.00 55.54           C
ATOM   898  CB  THR A 138      27.342  29.297  35.732  1.00 55.54           C
ATOM   899  OG1 THR A 138      27.916  28.110  36.292  1.00 55.73           O
ATOM   900  CG2 THR A 138      28.458  30.209  35.236  1.00 55.51           C
ATOM   901  C   THR A 138      25.984  31.326  36.223  1.00 56.87           C
ATOM   902  O   THR A 138      26.685  32.337  36.264  1.00 57.03           O
ATOM   903  N   VAL A 139      24.769  31.314  35.682  1.00 58.47           N
ATOM   904  CA  VAL A 139      24.190  32.516  35.087  1.00 60.06           C
ATOM   905  CB  VAL A 139      23.136  32.151  34.009  1.00 59.85           C
ATOM   906  CG1 VAL A 139      23.805  31.438  32.846  1.00 59.91           C
ATOM   907  CG2 VAL A 139      22.055  31.273  34.613  1.00 59.77           C
ATOM   908  C   VAL A 139      23.537  33.432  36.123  1.00 61.27           C
ATOM   909  O   VAL A 139      23.011  34.495  35.783  1.00 61.39           O
ATOM   910  N   LYS A 140      23.581  33.020  37.386  1.00 62.64           N
ATOM   911  CA  LYS A 140      22.987  33.797  38.471  1.00 64.06           C
ATOM   912  CB  LYS A 140      22.045  32.902  39.285  1.00 64.35           C
ATOM   913  CG  LYS A 140      21.287  33.610  40.403  1.00 64.87           C
ATOM   914  CD  LYS A 140      20.275  32.679  41.073  1.00 65.20           C
ATOM   915  CE  LYS A 140      20.948  31.483  41.739  1.00 65.27           C
ATOM   916  NZ  LYS A 140      21.879  31.897  42.826  1.00 65.54           N
ATOM   917  C   LYS A 140      24.071  34.378  39.379  1.00 64.96           C
ATOM   918  O   LYS A 140      23.778  35.104  40.331  1.00 65.26           O
ATOM   919  N   ARG A 141      25.323  34.057  39.070  1.00 65.90           N
ATOM   920  CA  ARG A 141      26.464  34.523  39.850  1.00 66.86           C
ATOM   921  CB  ARG A 141      27.653  33.584  39.639  1.00 67.34           C
ATOM   922  CG  ARG A 141      27.501  32.230  40.306  1.00 68.13           C
ATOM   923  CD  ARG A 141      27.641  32.357  41.813  1.00 68.85           C
ATOM   924  NE  ARG A 141      27.467  31.079  42.497  1.00 69.48           N
ATOM   925  CZ  ARG A 141      26.332  30.387  42.510  1.00 69.74           C
ATOM   926  NH1 ARG A 141      25.263  30.847  41.873  1.00 69.96           N
ATOM   927  NH2 ARG A 141      26.262  29.238  43.167  1.00 69.94           N
ATOM   928  C   ARG A 141      26.889  35.946  39.511  1.00 67.23           C
ATOM   929  O   ARG A 141      26.868  36.353  38.349  1.00 67.16           O
ATOM   930  N   SER A 142      27.283  36.695  40.537  1.00 67.70           N
ATOM   931  CA  SER A 142      27.733  38.069  40.354  1.00 68.23           C
ATOM   932  CB  SER A 142      27.953  38.742  41.713  1.00 68.35           C
ATOM   933  OG  SER A 142      28.985  38.101  42.441  1.00 68.33           O
ATOM   934  C   SER A 142      29.040  38.061  39.567  1.00 68.56           C
ATOM   935  O   SER A 142      29.280  38.931  38.731  1.00 68.56           O
ATOM   936  N   TYR A 143      29.878  37.067  39.845  1.00 68.92           N
ATOM   937  CA  TYR A 143      31.164  36.921  39.171  1.00 69.28           C
ATOM   938  CB  TYR A 143      31.829  35.609  39.605  1.00 69.43           C
ATOM   939  CG  TYR A 143      33.270  35.440  39.157  1.00 69.75           C
ATOM   940  CD1 TYR A 143      33.605  35.365  37.804  1.00 69.92           C
ATOM   941  CE1 TYR A 143      34.930  35.193  37.395  1.00 69.93           C
ATOM   942  CD2 TYR A 143      34.300  35.339  40.094  1.00 69.94           C
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Figure 10R

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ATOM   943  CE2 TYR A 143     35.628  35.165  39.697  1.00 69.89      C
ATOM   944  CZ  TYR A 143     35.935  35.093  38.346  1.00 69.96      C
ATOM   945  OH  TYR A 143     37.243  34.918  37.950  1.00 69.93      O
ATOM   946  C   TYR A 143     30.945  36.916  37.659  1.00 69.53      C
ATOM   947  O   TYR A 143     31.741  37.474  36.900  1.00 69.51      O
ATOM   948  N   THR A 144     29.857  36.286  37.229  1.00 69.65      N
ATOM   949  CA  THR A 144     29.539  36.207  35.811  1.00 70.00      C
ATOM   950  CB  THR A 144     28.400  35.200  35.553  1.00 69.84      C
ATOM   951  OG1 THR A 144     28.718  33.944  36.168  1.00 69.88      O
ATOM   952  CG2 THR A 144     28.210  34.987  34.056  1.00 69.88      C
ATOM   953  C   THR A 144     29.123  37.577  35.277  1.00 70.22      C
ATOM   954  O   THR A 144     29.803  38.149  34.424  1.00 70.09      O
ATOM   955  N   HIS A 145     28.011  38.096  35.794  1.00 70.56      N
ATOM   956  CA  HIS A 145     27.484  39.395  35.378  1.00 70.96      C
ATOM   957  CB  HIS A 145     26.435  39.893  36.380  1.00 71.08      C
ATOM   958  CG  HIS A 145     25.333  38.916  36.643  1.00 71.36      C
ATOM   959  CD2 HIS A 145     24.826  38.435  37.803  1.00 71.32      C
ATOM   960  ND1 HIS A 145     24.602  38.327  35.633  1.00 71.38      N
ATOM   961  CE1 HIS A 145     23.694  37.525  36.160  1.00 71.57      C
ATOM   962  NE2 HIS A 145     23.809  37.572  37.475  1.00 71.52      N
ATOM   963  C   HIS A 145     28.582  40.446  35.245  1.00 71.08      C
ATOM   964  O   HIS A 145     28.543  41.296  34.354  1.00 71.07      O
ATOM   965  N   GLU A 146     29.559  40.381  36.142  1.00 71.21      N
ATOM   966  CA  GLU A 146     30.671  41.321  36.139  1.00 71.44      C
ATOM   967  CB  GLU A 146     31.480  41.165  37.428  1.00 71.84      C
ATOM   968  CG  GLU A 146     30.672  41.443  38.688  1.00 72.39      C
ATOM   969  CD  GLU A 146     31.393  41.024  39.956  1.00 72.71      C
ATOM   970  OE1 GLU A 146     30.792  41.143  41.043  1.00 73.01      O
ATOM   971  OE2 GLU A 146     32.558  40.576  39.868  1.00 72.85      O
ATOM   972  C   GLU A 146     31.575  41.116  34.930  1.00 71.35      C
ATOM   973  O   GLU A 146     31.878  42.063  34.206  1.00 71.49      O
ATOM   974  N   LEU A 147     32.004  39.876  34.714  1.00 71.27      N
ATOM   975  CA  LEU A 147     32.874  39.556  33.589  1.00 71.04      C
ATOM   976  CB  LEU A 147     33.146  38.050  33.546  1.00 71.09      C
ATOM   977  CG  LEU A 147     34.138  37.538  32.498  1.00 71.03      C
ATOM   978  CD1 LEU A 147     35.511  38.141  32.744  1.00 70.98      C
ATOM   979  CD2 LEU A 147     34.213  36.021  32.574  1.00 71.22      C
ATOM   980  C   LEU A 147     32.232  40.000  32.277  1.00 70.90      C
ATOM   981  O   LEU A 147     32.914  40.466  31.364  1.00 70.81      O
ATOM   982  N   ILE A 148     30.914  39.855  32.198  1.00 70.62      N
ATOM   983  CA  ILE A 148     30.163  40.233  31.008  1.00 70.53      C
ATOM   984  CB  ILE A 148     28.669  39.878  31.172  1.00 70.38      C
ATOM   985  CG2 ILE A 148     27.858  40.466  30.025  1.00 70.25      C
ATOM   986  CG1 ILE A 148     28.506  38.358  31.229  1.00 70.30      C
ATOM   987  CD1 ILE A 148     27.075  37.894  31.422  1.00 70.22      C
ATOM   988  C   ILE A 148     30.285  41.723  30.701  1.00 70.59      C
ATOM   989  O   ILE A 148     30.228  42.135  29.543  1.00 70.52      O
ATOM   990  N   ALA A 149     30.457  42.527  31.743  1.00 70.67      N
ATOM   991  CA  ALA A 149     30.579  43.967  31.573  1.00 70.58      C
ATOM   992  CB  ALA A 149     29.961  44.681  32.769  1.00 70.60      C
ATOM   993  C   ALA A 149     32.034  44.392  31.402  1.00 70.54      C
ATOM   994  O   ALA A 149     32.323  45.395  30.747  1.00 70.64      O
ATOM   995  N   ARG A 150     32.948  43.620  31.979  1.00 70.38      N
ATOM   996  CA  ARG A 150     34.370  43.938  31.906  1.00 70.26      C
ATOM   997  CB  ARG A 150     35.140  43.138  32.964  1.00 70.67      C
ATOM   998  CG  ARG A 150     36.625  43.473  33.034  1.00 71.26      C
ATOM   999  CD  ARG A 150     37.341  42.765  34.186  1.00 71.83      C
ATOM  1000  NE  ARG A 150     36.910  43.228  35.505  1.00 72.23      N
```

Figure 10S

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ATOM   1001  CZ  ARG A 150      35.813  42.811  36.134  1.00 72.55           C
ATOM   1002  NH1 ARG A 150      35.017  41.907  35.572  1.00 72.75           N
ATOM   1003  NH2 ARG A 150      35.511  43.299  37.331  1.00 72.57           N
ATOM   1004  C   ARG A 150      35.024  43.735  30.536  1.00 69.94           C
ATOM   1005  O   ARG A 150      35.754  44.611  30.063  1.00 69.86           O
ATOM   1006  N   PHE A 151      34.773  42.595  29.895  1.00 69.42           N
ATOM   1007  CA  PHE A 151      35.380  42.329  28.591  1.00 68.83           C
ATOM   1008  CB  PHE A 151      36.232  41.055  28.644  1.00 68.80           C
ATOM   1009  CG  PHE A 151      37.376  41.128  29.616  1.00 68.86           C
ATOM   1010  CD1 PHE A 151      37.245  40.621  30.905  1.00 68.95           C
ATOM   1011  CD2 PHE A 151      38.583  41.714  29.247  1.00 68.94           C
ATOM   1012  CE1 PHE A 151      38.302  40.696  31.813  1.00 68.85           C
ATOM   1013  CE2 PHE A 151      39.645  41.794  30.148  1.00 68.87           C
ATOM   1014  CZ  PHE A 151      39.503  41.284  31.432  1.00 68.86           C
ATOM   1015  C   PHE A 151      34.400  42.221  27.426  1.00 68.31           C
ATOM   1016  O   PHE A 151      34.789  41.836  26.324  1.00 68.27           O
ATOM   1017  N   ALA A 152      33.139  42.564  27.661  1.00 67.70           N
ATOM   1018  CA  ALA A 152      32.136  42.498  26.605  1.00 67.16           C
ATOM   1019  CB  ALA A 152      31.309  41.231  26.757  1.00 67.17           C
ATOM   1020  C   ALA A 152      31.229  43.725  26.621  1.00 66.73           C
ATOM   1021  O   ALA A 152      30.010  43.613  26.510  1.00 66.67           O
ATOM   1022  N   ASN A 153      31.838  44.899  26.751  1.00 66.39           N
ATOM   1023  CA  ASN A 153      31.098  46.156  26.791  1.00 65.89           C
ATOM   1024  CB  ASN A 153      31.966  47.243  27.436  1.00 66.36           C
ATOM   1025  CG  ASN A 153      31.191  48.517  27.732  1.00 66.81           C
ATOM   1026  OD1 ASN A 153      31.761  49.509  28.191  1.00 66.98           O
ATOM   1027  ND2 ASN A 153      29.886  48.495  27.478  1.00 66.94           N
ATOM   1028  C   ASN A 153      30.669  46.600  25.392  1.00 65.27           C
ATOM   1029  O   ASN A 153      29.718  47.364  25.237  1.00 65.39           O
ATOM   1030  N   GLU A 154      31.369  46.111  24.374  1.00 64.45           N
ATOM   1031  CA  GLU A 154      31.063  46.476  22.997  1.00 63.52           C
ATOM   1032  CB  GLU A 154      32.366  46.632  22.204  1.00 64.22           C
ATOM   1033  CG  GLU A 154      33.491  45.686  22.626  1.00 65.05           C
ATOM   1034  CD  GLU A 154      33.119  44.220  22.493  1.00 65.51           C
ATOM   1035  OE1 GLU A 154      32.757  43.794  21.373  1.00 65.78           O
ATOM   1036  OE2 GLU A 154      33.193  43.495  23.510  1.00 65.61           O
ATOM   1037  C   GLU A 154      30.121  45.519  22.269  1.00 62.47           C
ATOM   1038  O   GLU A 154      29.863  45.687  21.074  1.00 62.51           O
ATOM   1039  N   CYS A 155      29.602  44.522  22.981  1.00 60.87           N
ATOM   1040  CA  CYS A 155      28.684  43.561  22.373  1.00 59.19           C
ATOM   1041  CB  CYS A 155      29.437  42.294  21.950  1.00 59.45           C
ATOM   1042  SG  CYS A 155      30.164  41.355  23.315  1.00 59.76           S
ATOM   1043  C   CYS A 155      27.564  43.192  23.337  1.00 57.82           C
ATOM   1044  O   CYS A 155      27.679  43.403  24.541  1.00 57.62           O
ATOM   1045  N   GLN A 156      26.477  42.645  22.802  1.00 56.31           N
ATOM   1046  CA  GLN A 156      25.353  42.249  23.637  1.00 54.79           C
ATOM   1047  CB  GLN A 156      24.024  42.538  22.932  1.00 55.37           C
ATOM   1048  CG  GLN A 156      23.782  41.739  21.671  1.00 56.39           C
ATOM   1049  CD  GLN A 156      22.406  41.995  21.084  1.00 57.13           C
ATOM   1050  OE1 GLN A 156      22.079  43.123  20.703  1.00 57.59           O
ATOM   1051  NE2 GLN A 156      21.590  40.946  21.011  1.00 57.49           N
ATOM   1052  C   GLN A 156      25.457  40.767  23.976  1.00 53.29           C
ATOM   1053  O   GLN A 156      25.692  39.929  23.107  1.00 53.00           O
ATOM   1054  N   ILE A 157      25.275  40.453  25.252  1.00 51.67           N
ATOM   1055  CA  ILE A 157      25.372  39.081  25.720  1.00 49.85           C
ATOM   1056  CB  ILE A 157      26.185  39.009  27.030  1.00 50.01           C
ATOM   1057  CG2 ILE A 157      26.243  37.575  27.537  1.00 50.23           C
ATOM   1058  CG1 ILE A 157      27.589  39.570  26.801  1.00 50.25           C
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Figure 10T

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ATOM  1059 CD1 ILE A 157    28.382  38.852  25.727  1.00 50.65      C
ATOM  1060 C   ILE A 157    24.021  38.430  25.958  1.00 48.42      C
ATOM  1061 O   ILE A 157    23.185  38.955  26.689  1.00 48.14      O
ATOM  1062 N   GLU A 158    23.819  37.279  25.328  1.00 46.69      N
ATOM  1063 CA  GLU A 158    22.589  36.518  25.481  1.00 45.32      C
ATOM  1064 CB  GLU A 158    22.104  35.996  24.127  1.00 45.68      C
ATOM  1065 CG  GLU A 158    21.695  37.070  23.136  1.00 46.58      C
ATOM  1066 CD  GLU A 158    20.560  37.931  23.652  1.00 47.34      C
ATOM  1067 OE1 GLU A 158    19.576  37.369  24.179  1.00 47.28      O
ATOM  1068 OE2 GLU A 158    20.650  39.169  23.525  1.00 48.19      O
ATOM  1069 C   GLU A 158    22.920  35.336  26.385  1.00 43.98      C
ATOM  1070 O   GLU A 158    23.606  34.407  25.963  1.00 43.50      O
ATOM  1071 N   MET A 159    22.446  35.378  27.626  1.00 42.74      N
ATOM  1072 CA  MET A 159    22.711  34.295  28.570  1.00 41.56      C
ATOM  1073 CB  MET A 159    22.798  34.815  30.004  1.00 42.39      C
ATOM  1074 CG  MET A 159    24.088  35.514  30.371  1.00 44.11      C
ATOM  1075 SD  MET A 159    24.267  35.526  32.176  1.00 46.60      S
ATOM  1076 CE  MET A 159    22.851  36.541  32.649  1.00 46.03      C
ATOM  1077 C   MET A 159    21.648  33.218  28.532  1.00 40.26      C
ATOM  1078 O   MET A 159    20.464  33.501  28.365  1.00 39.98      O
ATOM  1079 N   LEU A 160    22.083  31.978  28.704  1.00 38.69      N
ATOM  1080 CA  LEU A 160    21.172  30.848  28.721  1.00 37.59      C
ATOM  1081 CB  LEU A 160    21.018  30.279  27.305  1.00 37.60      C
ATOM  1082 CG  LEU A 160    19.784  29.422  27.024  1.00 37.90      C
ATOM  1083 CD1 LEU A 160    19.650  29.202  25.519  1.00 37.83      C
ATOM  1084 CD2 LEU A 160    19.890  28.097  27.761  1.00 37.80      C
ATOM  1085 C   LEU A 160    21.750  29.800  29.677  1.00 36.65      C
ATOM  1086 O   LEU A 160    22.753  29.151  29.374  1.00 36.13      O
ATOM  1087 N   GLY A 161    21.125  29.663  30.844  1.00 35.74      N
ATOM  1088 CA  GLY A 161    21.586  28.699  31.831  1.00 34.53      C
ATOM  1089 C   GLY A 161    20.761  27.429  31.760  1.00 33.81      C
ATOM  1090 O   GLY A 161    19.531  27.483  31.773  1.00 33.71      O
ATOM  1091 N   SER A 162    21.424  26.281  31.688  1.00 32.70      N
ATOM  1092 CA  SER A 162    20.701  25.018  31.599  1.00 31.67      C
ATOM  1093 CB  SER A 162    20.570  24.587  30.134  1.00 30.98      C
ATOM  1094 OG  SER A 162    19.993  23.293  30.042  1.00 30.57      O
ATOM  1095 C   SER A 162    21.317  23.873  32.386  1.00 31.01      C
ATOM  1096 O   SER A 162    22.365  23.346  32.016  1.00 30.76      O
ATOM  1097 N   ALA A 163    20.650  23.477  33.464  1.00 30.33      N
ATOM  1098 CA  ALA A 163    21.125  22.369  34.273  1.00 29.58      C
ATOM  1099 CB  ALA A 163    20.385  22.341  35.603  1.00 30.07      C
ATOM  1100 C   ALA A 163    20.856  21.080  33.489  1.00 29.44      C
ATOM  1101 O   ALA A 163    21.569  20.089  33.631  1.00 28.92      O
ATOM  1102 N   GLU A 164    19.825  21.106  32.649  1.00 29.32      N
ATOM  1103 CA  GLU A 164    19.476  19.936  31.853  1.00 29.78      C
ATOM  1104 CB  GLU A 164    18.172  20.184  31.095  1.00 31.44      C
ATOM  1105 CG  GLU A 164    17.655  18.951  30.371  1.00 34.82      C
ATOM  1106 CD  GLU A 164    16.325  19.187  29.679  1.00 36.46      C
ATOM  1107 OE1 GLU A 164    15.678  20.222  29.958  1.00 38.07      O
ATOM  1108 OE2 GLU A 164    15.924  18.327  28.864  1.00 37.79      O
ATOM  1109 C   GLU A 164    20.582  19.575  30.859  1.00 29.30      C
ATOM  1110 O   GLU A 164    20.847  18.399  30.596  1.00 28.77      O
ATOM  1111 N   MET A 165    21.232  20.587  30.300  1.00 28.45      N
ATOM  1112 CA  MET A 165    22.298  20.317  29.345  1.00 28.20      C
ATOM  1113 CB  MET A 165    22.778  21.620  28.710  1.00 28.91      C
ATOM  1114 CG  MET A 165    23.570  21.398  27.431  1.00 30.59      C
ATOM  1115 SD  MET A 165    24.035  22.940  26.620  1.00 31.94      S
ATOM  1116 CE  MET A 165    22.494  23.418  25.882  1.00 31.97      C
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Figure 10U

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ATOM   1117  C   MET A 165      23.454  19.606  30.050  1.00 27.54           C
ATOM   1118  O   MET A 165      24.131  18.758  29.463  1.00 27.24           O
ATOM   1119  N   VAL A 166      23.678  19.952  31.314  1.00 26.73           N
ATOM   1120  CA  VAL A 166      24.740  19.311  32.073  1.00 26.74           C
ATOM   1121  CB  VAL A 166      24.841  19.883  33.500  1.00 26.61           C
ATOM   1122  CG1 VAL A 166      25.928  19.145  34.277  1.00 26.96           C
ATOM   1123  CG2 VAL A 166      25.149  21.373  33.441  1.00 26.49           C
ATOM   1124  C   VAL A 166      24.424  17.820  32.152  1.00 27.07           C
ATOM   1125  O   VAL A 166      25.301  16.980  31.972  1.00 26.02           O
ATOM   1126  N   GLU A 167      23.158  17.506  32.417  1.00 27.89           N
ATOM   1127  CA  GLU A 167      22.714  16.121  32.517  1.00 29.12           C
ATOM   1128  CB  GLU A 167      21.260  16.062  33.002  1.00 31.04           C
ATOM   1129  CG  GLU A 167      21.099  16.378  34.471  1.00 34.37           C
ATOM   1130  CD  GLU A 167      22.033  15.552  35.344  1.00 36.89           C
ATOM   1131  OE1 GLU A 167      22.130  14.321  35.130  1.00 38.46           O
ATOM   1132  OE2 GLU A 167      22.675  16.130  36.249  1.00 38.74           O
ATOM   1133  C   GLU A 167      22.842  15.390  31.189  1.00 28.28           C
ATOM   1134  O   GLU A 167      23.150  14.200  31.153  1.00 28.26           O
ATOM   1135  N   LEU A 168      22.598  16.100  30.095  1.00 28.21           N
ATOM   1136  CA  LEU A 168      22.712  15.494  28.779  1.00 28.05           C
ATOM   1137  CB  LEU A 168      22.265  16.487  27.697  1.00 28.07           C
ATOM   1138  CG  LEU A 168      20.756  16.747  27.683  1.00 28.26           C
ATOM   1139  CD1 LEU A 168      20.422  17.814  26.662  1.00 28.45           C
ATOM   1140  CD2 LEU A 168      20.025  15.452  27.366  1.00 28.49           C
ATOM   1141  C   LEU A 168      24.163  15.077  28.568  1.00 27.93           C
ATOM   1142  O   LEU A 168      24.438  13.999  28.037  1.00 28.11           O
ATOM   1143  N   ALA A 169      25.089  15.926  29.007  1.00 27.73           N
ATOM   1144  CA  ALA A 169      26.515  15.632  28.873  1.00 28.12           C
ATOM   1145  CB  ALA A 169      27.358  16.852  29.288  1.00 27.69           C
ATOM   1146  C   ALA A 169      26.859  14.426  29.746  1.00 28.18           C
ATOM   1147  O   ALA A 169      27.572  13.519  29.311  1.00 28.29           O
ATOM   1148  N   GLU A 170      26.357  14.415  30.978  1.00 28.76           N
ATOM   1149  CA  GLU A 170      26.610  13.285  31.873  1.00 29.18           C
ATOM   1150  CB  GLU A 170      25.898  13.480  33.218  1.00 29.14           C
ATOM   1151  CG  GLU A 170      26.581  14.460  34.167  1.00 29.02           C
ATOM   1152  CD  GLU A 170      27.862  13.903  34.788  1.00 29.97           C
ATOM   1153  OE1 GLU A 170      28.793  14.700  35.045  1.00 29.30           O
ATOM   1154  OE2 GLU A 170      27.939  12.676  35.032  1.00 30.01           O
ATOM   1155  C   GLU A 170      26.099  12.011  31.205  1.00 29.51           C
ATOM   1156  O   GLU A 170      26.824  11.025  31.090  1.00 29.71           O
ATOM   1157  N   ALA A 171      24.848  12.042  30.752  1.00 29.94           N
ATOM   1158  CA  ALA A 171      24.253  10.883  30.094  1.00 30.26           C
ATOM   1159  CB  ALA A 171      22.868  11.234  29.572  1.00 30.29           C
ATOM   1160  C   ALA A 171      25.124  10.394  28.947  1.00 30.81           C
ATOM   1161  O   ALA A 171      25.412   9.201  28.834  1.00 31.13           O
ATOM   1162  N   LYS A 172      25.546  11.316  28.091  1.00 31.06           N
ATOM   1163  CA  LYS A 172      26.366  10.947  26.950  1.00 32.12           C
ATOM   1164  CB  LYS A 172      26.795  12.192  26.171  1.00 32.06           C
ATOM   1165  CG  LYS A 172      27.626  11.871  24.940  1.00 32.46           C
ATOM   1166  CD  LYS A 172      28.013  13.136  24.180  1.00 32.50           C
ATOM   1167  CE  LYS A 172      28.815  12.800  22.932  1.00 33.01           C
ATOM   1168  NZ  LYS A 172      29.159  14.022  22.167  1.00 32.96           N
ATOM   1169  C   LYS A 172      27.597  10.131  27.326  1.00 32.64           C
ATOM   1170  O   LYS A 172      27.829   9.062  26.757  1.00 32.92           O
ATOM   1171  N   LEU A 173      28.387  10.620  28.276  1.00 33.14           N
ATOM   1172  CA  LEU A 173      29.587   9.897  28.669  1.00 34.31           C
ATOM   1173  CB  LEU A 173      30.552  10.812  29.433  1.00 34.17           C
ATOM   1174  CG  LEU A 173      31.093  12.078  28.747  1.00 34.37           C
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Figure 10V

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ATOM  1175 CD1 LEU A 173    32.576  12.212  29.062  1.00 33.96      C
ATOM  1176 CD2 LEU A 173    30.880  12.025  27.247  1.00 34.33      C
ATOM  1177 C   LEU A 173    29.278   8.653  29.496  1.00 35.30      C
ATOM  1178 O   LEU A 173    30.172   7.870  29.805  1.00 35.42      O
ATOM  1179 N   HIS A 174    28.015   8.473  29.864  1.00 36.72      N
ATOM  1180 CA  HIS A 174    27.630   7.293  30.626  1.00 38.16      C
ATOM  1181 CB  HIS A 174    26.560   7.644  31.664  1.00 37.76      C
ATOM  1182 CG  HIS A 174    27.124   8.213  32.929  1.00 37.39      C
ATOM  1183 CD2 HIS A 174    27.348   9.494  33.308  1.00 37.15      C
ATOM  1184 ND1 HIS A 174    27.602   7.422  33.953  1.00 37.82      N
ATOM  1185 CE1 HIS A 174    28.095   8.192  34.907  1.00 37.44      C
ATOM  1186 NE2 HIS A 174    27.955   9.453  34.540  1.00 37.12      N
ATOM  1187 C   HIS A 174    27.130   6.219  29.669  1.00 39.31      C
ATOM  1188 O   HIS A 174    26.810   5.108  30.083  1.00 39.72      O
ATOM  1189 N   GLY A 175    27.073   6.560  28.384  1.00 40.42      N
ATOM  1190 CA  GLY A 175    26.639   5.597  27.387  1.00 41.81      C
ATOM  1191 C   GLY A 175    25.287   5.845  26.747  1.00 43.00      C
ATOM  1192 O   GLY A 175    24.886   5.105  25.846  1.00 43.03      O
ATOM  1193 N   GLU A 176    24.571   6.868  27.204  1.00 43.77      N
ATOM  1194 CA  GLU A 176    23.266   7.173  26.629  1.00 45.02      C
ATOM  1195 CB  GLU A 176    22.324   7.762  27.686  1.00 46.03      C
ATOM  1196 CG  GLU A 176    21.921   6.795  28.792  1.00 47.96      C
ATOM  1197 CD  GLU A 176    22.955   6.689  29.898  1.00 49.25      C
ATOM  1198 OE1 GLU A 176    23.169   7.694  30.614  1.00 49.83      O
ATOM  1199 OE2 GLU A 176    23.552   5.601  30.055  1.00 50.12      O
ATOM  1200 C   GLU A 176    23.413   8.153  25.474  1.00 45.17      C
ATOM  1201 O   GLU A 176    24.327   8.975  25.459  1.00 45.70      O
ATOM  1202 N   ASP A 177    22.512   8.059  24.503  1.00 45.24      N
ATOM  1203 CA  ASP A 177    22.545   8.938  23.342  1.00 44.89      C
ATOM  1204 CB  ASP A 177    21.869   8.253  22.157  1.00 46.19      C
ATOM  1205 CG  ASP A 177    22.460   6.882  21.871  1.00 47.31      C
ATOM  1206 OD1 ASP A 177    23.559   6.818  21.272  1.00 47.70      O
ATOM  1207 OD2 ASP A 177    21.831   5.873  22.267  1.00 48.01      O
ATOM  1208 C   ASP A 177    21.833  10.238  23.672  1.00 43.98      C
ATOM  1209 O   ASP A 177    20.814  10.243  24.357  1.00 44.07      O
ATOM  1210 N   VAL A 178    22.381  11.342  23.186  1.00 42.87      N
ATOM  1211 CA  VAL A 178    21.800  12.649  23.441  1.00 41.57      C
ATOM  1212 CB  VAL A 178    22.852  13.765  23.229  1.00 41.43      C
ATOM  1213 CG1 VAL A 178    22.253  15.120  23.567  1.00 40.77      C
ATOM  1214 CG2 VAL A 178    24.085  13.484  24.083  1.00 41.33      C
ATOM  1215 C   VAL A 178    20.608  12.913  22.524  1.00 40.74      C
ATOM  1216 O   VAL A 178    20.715  12.801  21.305  1.00 40.65      O
ATOM  1217 N   SER A 179    19.471  13.260  23.118  1.00 40.12      N
ATOM  1218 CA  SER A 179    18.271  13.564  22.346  1.00 39.22      C
ATOM  1219 CB  SER A 179    17.032  13.517  23.234  1.00 39.19      C
ATOM  1220 OG  SER A 179    15.955  14.187  22.604  1.00 39.12      O
ATOM  1221 C   SER A 179    18.397  14.957  21.751  1.00 38.78      C
ATOM  1222 O   SER A 179    18.419  15.950  22.482  1.00 38.57      O
ATOM  1223 N   LEU A 180    18.480  15.036  20.427  1.00 38.11      N
ATOM  1224 CA  LEU A 180    18.602  16.330  19.772  1.00 37.12      C
ATOM  1225 CB  LEU A 180    18.859  16.153  18.276  1.00 37.25      C
ATOM  1226 CG  LEU A 180    20.159  15.430  17.903  1.00 37.36      C
ATOM  1227 CD1 LEU A 180    20.354  15.483  16.394  1.00 37.56      C
ATOM  1228 CD2 LEU A 180    21.344  16.082  18.615  1.00 37.57      C
ATOM  1229 C   LEU A 180    17.355  17.173  19.995  1.00 36.72      C
ATOM  1230 O   LEU A 180    17.433  18.398  20.045  1.00 36.33      O
ATOM  1231 N   ASP A 181    16.203  16.523  20.136  1.00 36.44      N
ATOM  1232 CA  ASP A 181    14.966  17.256  20.366  1.00 36.07      C
```

Figure 10W

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ATOM  1233  CB  ASP A 181     13.754  16.319  20.311  1.00 37.55      C
ATOM  1234  CG  ASP A 181     13.486  15.790  18.909  1.00 38.95      C
ATOM  1235  OD1 ASP A 181     13.589  16.570  17.937  1.00 39.74      O
ATOM  1236  OD2 ASP A 181     13.158  14.594  18.777  1.00 40.38      O
ATOM  1237  C   ASP A 181     15.014  17.971  21.714  1.00 34.99      C
ATOM  1238  O   ASP A 181     14.491  19.074  21.859  1.00 34.62      O
ATOM  1239  N   ALA A 182     15.638  17.337  22.702  1.00 34.20      N
ATOM  1240  CA  ALA A 182     15.766  17.939  24.026  1.00 33.44      C
ATOM  1241  CB  ALA A 182     16.388  16.937  25.003  1.00 33.26      C
ATOM  1242  C   ALA A 182     16.645  19.186  23.910  1.00 32.88      C
ATOM  1243  O   ALA A 182     16.362  20.216  24.514  1.00 32.37      O
ATOM  1244  N   LEU A 183     17.714  19.085  23.124  1.00 32.52      N
ATOM  1245  CA  LEU A 183     18.614  20.214  22.915  1.00 31.97      C
ATOM  1246  CB  LEU A 183     19.823  19.796  22.080  1.00 32.53      C
ATOM  1247  CG  LEU A 183     21.089  19.365  22.816  1.00 33.44      C
ATOM  1248  CD1 LEU A 183     22.184  19.088  21.785  1.00 33.67      C
ATOM  1249  CD2 LEU A 183     21.533  20.463  23.787  1.00 33.50      C
ATOM  1250  C   LEU A 183     17.913  21.366  22.213  1.00 31.47      C
ATOM  1251  O   LEU A 183     18.060  22.524  22.609  1.00 31.07      O
ATOM  1252  N   LYS A 184     17.160  21.050  21.163  1.00 30.86      N
ATOM  1253  CA  LYS A 184     16.443  22.075  20.413  1.00 31.16      C
ATOM  1254  CB  LYS A 184     15.651  21.445  19.262  1.00 31.63      C
ATOM  1255  CG  LYS A 184     16.513  20.868  18.158  1.00 32.93      C
ATOM  1256  CD  LYS A 184     15.675  20.111  17.139  1.00 33.75      C
ATOM  1257  CE  LYS A 184     16.556  19.416  16.115  1.00 34.92      C
ATOM  1258  NZ  LYS A 184     15.750  18.568  15.178  1.00 35.78      N
ATOM  1259  C   LYS A 184     15.487  22.824  21.328  1.00 30.89      C
ATOM  1260  O   LYS A 184     15.307  24.033  21.199  1.00 30.37      O
ATOM  1261  N   ARG A 185     14.869  22.090  22.244  1.00 30.97      N
ATOM  1262  CA  ARG A 185     13.926  22.680  23.183  1.00 31.66      C
ATOM  1263  CB  ARG A 185     13.260  21.576  24.011  1.00 32.95      C
ATOM  1264  CG  ARG A 185     12.273  22.095  25.045  1.00 35.19      C
ATOM  1265  CD  ARG A 185     11.071  22.763  24.385  1.00 36.95      C
ATOM  1266  NE  ARG A 185     10.276  23.497  25.366  1.00 38.48      N
ATOM  1267  CZ  ARG A 185     10.678  24.616  25.959  1.00 39.27      C
ATOM  1268  NH1 ARG A 185     11.864  25.138  25.668  1.00 39.25      N
ATOM  1269  NH2 ARG A 185      9.901  25.206  26.857  1.00 40.18      N
ATOM  1270  C   ARG A 185     14.667  23.645  24.101  1.00 30.92      C
ATOM  1271  O   ARG A 185     14.239  24.781  24.313  1.00 30.74      O
ATOM  1272  N   ILE A 186     15.789  23.186  24.642  1.00 30.14      N
ATOM  1273  CA  ILE A 186     16.585  24.022  25.528  1.00 29.32      C
ATOM  1274  CB  ILE A 186     17.832  23.252  26.037  1.00 29.04      C
ATOM  1275  CG2 ILE A 186     18.741  24.190  26.829  1.00 29.20      C
ATOM  1276  CG1 ILE A 186     17.389  22.058  26.894  1.00 29.51      C
ATOM  1277  CD1 ILE A 186     18.534  21.148  27.330  1.00 29.37      C
ATOM  1278  C   ILE A 186     17.037  25.285  24.792  1.00 28.71      C
ATOM  1279  O   ILE A 186     17.015  26.380  25.351  1.00 28.31      O
ATOM  1280  N   LEU A 187     17.435  25.130  23.532  1.00 28.36      N
ATOM  1281  CA  LEU A 187     17.911  26.257  22.733  1.00 28.42      C
ATOM  1282  CB  LEU A 187     18.998  25.772  21.757  1.00 28.23      C
ATOM  1283  CG  LEU A 187     20.268  25.207  22.409  1.00 28.51      C
ATOM  1284  CD1 LEU A 187     21.125  24.483  21.376  1.00 28.72      C
ATOM  1285  CD2 LEU A 187     21.049  26.337  23.051  1.00 28.48      C
ATOM  1286  C   LEU A 187     16.814  26.996  21.956  1.00 28.77      C
ATOM  1287  O   LEU A 187     17.105  27.913  21.189  1.00 27.81      O
ATOM  1288  N   ARG A 188     15.559  26.611  22.173  1.00 29.44      N
ATOM  1289  CA  ARG A 188     14.437  27.232  21.470  1.00 30.59      C
ATOM  1290  CB  ARG A 188     13.096  26.759  22.066  1.00 31.00      C
```

Figure 10X

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ATOM  1291  CG  ARG A 188     11.880  27.044  21.161  1.00 31.92      C
ATOM  1292  CD  ARG A 188     10.591  26.415  21.694  1.00 32.72      C
ATOM  1293  NE  ARG A 188     10.065  27.111  22.869  1.00 33.40      N
ATOM  1294  CZ  ARG A 188      8.896  26.834  23.440  1.00 33.80      C
ATOM  1295  NH1 ARG A 188      8.127  25.871  22.951  1.00 34.90      N
ATOM  1296  NH2 ARG A 188      8.486  27.525  24.492  1.00 34.07      N
ATOM  1297  C   ARG A 188     14.522  28.761  21.479  1.00 31.15      C
ATOM  1298  O   ARG A 188     14.384  29.394  20.437  1.00 31.37      O
ATOM  1299  N   PRO A 189     14.778  29.373  22.652  1.00 31.69      N
ATOM  1300  CD  PRO A 189     15.085  28.750  23.953  1.00 31.58      C
ATOM  1301  CA  PRO A 189     14.877  30.835  22.741  1.00 32.00      C
ATOM  1302  CB  PRO A 189     15.460  31.055  24.134  1.00 32.34      C
ATOM  1303  CG  PRO A 189     14.931  29.907  24.908  1.00 32.12      C
ATOM  1304  C   PRO A 189     15.781  31.423  21.661  1.00 32.69      C
ATOM  1305  O   PRO A 189     15.444  32.428  21.024  1.00 33.41      O
ATOM  1306  N   TRP A 190     16.937  30.795  21.467  1.00 32.33      N
ATOM  1307  CA  TRP A 190     17.902  31.251  20.478  1.00 32.66      C
ATOM  1308  CB  TRP A 190     19.276  30.637  20.767  1.00 31.96      C
ATOM  1309  CG  TRP A 190     19.946  31.238  21.972  1.00 31.74      C
ATOM  1310  CD2 TRP A 190     21.261  30.942  22.461  1.00 31.19      C
ATOM  1311  CE2 TRP A 190     21.475  31.752  23.597  1.00 31.14      C
ATOM  1312  CE3 TRP A 190     22.278  30.070  22.048  1.00 31.17      C
ATOM  1313  CD1 TRP A 190     19.432  32.187  22.808  1.00 31.47      C
ATOM  1314  NE1 TRP A 190     20.343  32.502  23.786  1.00 31.75      N
ATOM  1315  CZ2 TRP A 190     22.666  31.719  24.327  1.00 30.64      C
ATOM  1316  CZ3 TRP A 190     23.468  30.038  22.777  1.00 30.63      C
ATOM  1317  CH2 TRP A 190     23.647  30.858  23.903  1.00 30.76      C
ATOM  1318  C   TRP A 190     17.473  30.936  19.053  1.00 32.80      C
ATOM  1319  O   TRP A 190     17.678  31.739  18.151  1.00 33.14      O
ATOM  1320  N   LEU A 191     16.875  29.769  18.853  1.00 33.23      N
ATOM  1321  CA  LEU A 191     16.420  29.384  17.525  1.00 34.12      C
ATOM  1322  CB  LEU A 191     15.997  27.913  17.514  1.00 34.10      C
ATOM  1323  CG  LEU A 191     17.133  26.920  17.767  1.00 34.63      C
ATOM  1324  CD1 LEU A 191     16.571  25.512  17.926  1.00 34.77      C
ATOM  1325  CD2 LEU A 191     18.124  26.985  16.605  1.00 34.84      C
ATOM  1326  C   LEU A 191     15.264  30.262  17.047  1.00 34.32      C
ATOM  1327  O   LEU A 191     14.943  30.270  15.864  1.00 34.60      O
ATOM  1328  N   ARG A 192     14.640  31.000  17.962  1.00 34.66      N
ATOM  1329  CA  ARG A 192     13.532  31.879  17.584  1.00 35.36      C
ATOM  1330  CB  ARG A 192     12.417  31.827  18.630  1.00 35.21      C
ATOM  1331  CG  ARG A 192     11.568  30.569  18.575  1.00 34.86      C
ATOM  1332  CD  ARG A 192     10.556  30.560  19.709  1.00 34.91      C
ATOM  1333  NE  ARG A 192      9.624  29.440  19.608  1.00 35.35      N
ATOM  1334  CZ  ARG A 192      8.670  29.181  20.500  1.00 34.80      C
ATOM  1335  NH1 ARG A 192      8.528  29.960  21.563  1.00 34.29      N
ATOM  1336  NH2 ARG A 192      7.851  28.152  20.318  1.00 34.13      N
ATOM  1337  C   ARG A 192     13.966  33.328  17.393  1.00 35.93      C
ATOM  1338  O   ARG A 192     13.130  34.204  17.168  1.00 36.00      O
ATOM  1339  N   MET A 193     15.270  33.579  17.479  1.00 36.28      N
ATOM  1340  CA  MET A 193     15.797  34.930  17.316  1.00 36.54      C
ATOM  1341  CB  MET A 193     17.139  35.070  18.045  1.00 36.79      C
ATOM  1342  CG  MET A 193     17.038  35.165  19.564  1.00 36.88      C
ATOM  1343  SD  MET A 193     18.669  35.278  20.352  1.00 37.53      S
ATOM  1344  CE  MET A 193     19.079  37.031  20.122  1.00 36.86      C
ATOM  1345  C   MET A 193     15.987  35.306  15.848  1.00 36.67      C
ATOM  1346  O   MET A 193     16.368  34.467  15.025  1.00 36.46      O
ATOM  1347  N   LYS A 194     15.715  36.570  15.526  1.00 37.01      N
ATOM  1348  CA  LYS A 194     15.889  37.067  14.163  1.00 37.69      C
```

Figure 10Y

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ATOM  1349  CB  LYS A 194      15.478  38.545  14.064  1.00 38.05      C
ATOM  1350  CG  LYS A 194      15.613  39.121  12.654  1.00 38.80      C
ATOM  1351  CD  LYS A 194      16.261  40.515  12.623  1.00 39.92      C
ATOM  1352  CE  LYS A 194      15.284  41.663  12.887  1.00 40.54      C
ATOM  1353  NZ  LYS A 194      14.817  41.801  14.299  1.00 41.22      N
ATOM  1354  C   LYS A 194      17.374  36.928  13.832  1.00 37.73      C
ATOM  1355  O   LYS A 194      17.757  36.399  12.787  1.00 37.39      O
ATOM  1356  N   GLU A 195      18.206  37.413  14.744  1.00 38.33      N
ATOM  1357  CA  GLU A 195      19.650  37.332  14.574  1.00 38.43      C
ATOM  1358  CB  GLU A 195      20.248  38.722  14.361  1.00 39.41      C
ATOM  1359  CG  GLU A 195      21.766  38.698  14.281  1.00 41.23      C
ATOM  1360  CD  GLU A 195      22.348  39.961  13.690  1.00 42.54      C
ATOM  1361  OE1 GLU A 195      21.953  41.066  14.125  1.00 43.29      O
ATOM  1362  OE2 GLU A 195      23.211  39.844  12.792  1.00 43.45      O
ATOM  1363  C   GLU A 195      20.268  36.688  15.810  1.00 37.55      C
ATOM  1364  O   GLU A 195      20.596  37.368  16.781  1.00 37.40      O
ATOM  1365  N   PRO A 196      20.422  35.358  15.792  1.00 36.88      N
ATOM  1366  CD  PRO A 196      20.121  34.417  14.697  1.00 37.02      C
ATOM  1367  CA  PRO A 196      21.006  34.659  16.940  1.00 36.26      C
ATOM  1368  CB  PRO A 196      20.744  33.191  16.611  1.00 36.49      C
ATOM  1369  CG  PRO A 196      20.877  33.165  15.122  1.00 37.04      C
ATOM  1370  C   PRO A 196      22.491  34.973  17.078  1.00 35.39      C
ATOM  1371  O   PRO A 196      23.105  35.530  16.166  1.00 35.42      O
ATOM  1372  N   PRO A 197      23.089  34.626  18.228  1.00 34.89      N
ATOM  1373  CD  PRO A 197      22.518  33.900  19.374  1.00 34.65      C
ATOM  1374  CA  PRO A 197      24.517  34.894  18.438  1.00 34.16      C
ATOM  1375  CB  PRO A 197      24.789  34.288  19.820  1.00 34.06      C
ATOM  1376  CG  PRO A 197      23.457  34.284  20.480  1.00 34.48      C
ATOM  1377  C   PRO A 197      25.334  34.192  17.366  1.00 33.22      C
ATOM  1378  O   PRO A 197      25.018  33.067  16.991  1.00 33.54      O
ATOM  1379  N   ASP A 198      26.376  34.838  16.857  1.00 32.64      N
ATOM  1380  CA  ASP A 198      27.200  34.173  15.861  1.00 32.00      C
ATOM  1381  CB  ASP A 198      27.669  35.169  14.782  1.00 32.92      C
ATOM  1382  CG  ASP A 198      28.741  36.136  15.269  1.00 34.20      C
ATOM  1383  OD1 ASP A 198      28.889  36.334  16.497  1.00 34.32      O
ATOM  1384  OD2 ASP A 198      29.433  36.718  14.394  1.00 34.48      O
ATOM  1385  C   ASP A 198      28.379  33.517  16.590  1.00 30.70      C
ATOM  1386  O   ASP A 198      29.151  32.754  16.008  1.00 30.48      O
ATOM  1387  N   THR A 199      28.477  33.797  17.885  1.00 29.73      N
ATOM  1388  CA  THR A 199      29.541  33.245  18.728  1.00 28.32      C
ATOM  1389  CB  THR A 199      30.609  34.317  19.009  1.00 28.44      C
ATOM  1390  OG1 THR A 199      31.040  34.892  17.767  1.00 28.45      O
ATOM  1391  CG2 THR A 199      31.817  33.703  19.712  1.00 27.68      C
ATOM  1392  C   THR A 199      28.925  32.774  20.050  1.00 27.54      C
ATOM  1393  O   THR A 199      28.258  33.544  20.731  1.00 27.62      O
ATOM  1394  N   VAL A 200      29.137  31.509  20.408  1.00 26.67      N
ATOM  1395  CA  VAL A 200      28.573  30.975  21.645  1.00 25.45      C
ATOM  1396  CB  VAL A 200      27.603  29.794  21.368  1.00 25.29      C
ATOM  1397  CG1 VAL A 200      27.103  29.205  22.688  1.00 24.41      C
ATOM  1398  CG2 VAL A 200      26.410  30.273  20.533  1.00 25.16      C
ATOM  1399  C   VAL A 200      29.665  30.485  22.586  1.00 24.96      C
ATOM  1400  O   VAL A 200      30.457  29.615  22.228  1.00 25.00      O
ATOM  1401  N   VAL A 201      29.692  31.050  23.787  1.00 24.00      N
ATOM  1402  CA  VAL A 201      30.672  30.680  24.803  1.00 24.07      C
ATOM  1403  CB  VAL A 201      30.931  31.850  25.784  1.00 23.91      C
ATOM  1404  CG1 VAL A 201      31.872  31.401  26.907  1.00 23.25      C
ATOM  1405  CG2 VAL A 201      31.527  33.032  25.035  1.00 23.70      C
ATOM  1406  C   VAL A 201      30.151  29.506  25.620  1.00 23.96      C
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Figure 10Z

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ATOM  1407  O   VAL A 201     29.044  29.551  26.144  1.00 24.03      O
ATOM  1408  N   LEU A 202     30.937  28.445  25.711  1.00 24.28      N
ATOM  1409  CA  LEU A 202     30.531  27.304  26.519  1.00 24.52      C
ATOM  1410  CB  LEU A 202     31.091  26.010  25.927  1.00 24.85      C
ATOM  1411  CG  LEU A 202     30.634  25.793  24.479  1.00 24.66      C
ATOM  1412  CD1 LEU A 202     31.126  24.450  23.954  1.00 25.52      C
ATOM  1413  CD2 LEU A 202     29.115  25.869  24.418  1.00 24.68      C
ATOM  1414  C   LEU A 202     31.123  27.596  27.890  1.00 24.97      C
ATOM  1415  O   LEU A 202     32.318  27.377  28.124  1.00 25.27      O
ATOM  1416  N   GLY A 203     30.283  28.132  28.772  1.00 25.47      N
ATOM  1417  CA  GLY A 203     30.708  28.498  30.114  1.00 26.68      C
ATOM  1418  C   GLY A 203     30.468  27.425  31.157  1.00 27.26      C
ATOM  1419  O   GLY A 203     30.282  27.711  32.337  1.00 28.58      O
ATOM  1420  N   CYS A 204     30.441  26.182  30.704  1.00 27.73      N
ATOM  1421  CA  CYS A 204     30.273  25.034  31.582  1.00 27.40      C
ATOM  1422  CB  CYS A 204     28.824  24.551  31.568  1.00 28.28      C
ATOM  1423  SG  CYS A 204     28.483  23.277  32.788  1.00 29.75      S
ATOM  1424  C   CYS A 204     31.200  23.998  30.959  1.00 26.65      C
ATOM  1425  O   CYS A 204     31.088  23.705  29.768  1.00 26.53      O
ATOM  1426  N   THR A 205     32.130  23.455  31.740  1.00 25.96      N
ATOM  1427  CA  THR A 205     33.072  22.481  31.188  1.00 25.54      C
ATOM  1428  CB  THR A 205     34.179  22.112  32.213  1.00 25.97      C
ATOM  1429  OG1 THR A 205     33.604  21.417  33.326  1.00 25.47      O
ATOM  1430  CG2 THR A 205     34.866  23.376  32.720  1.00 26.26      C
ATOM  1431  C   THR A 205     32.398  21.209  30.671  1.00 25.02      C
ATOM  1432  O   THR A 205     33.020  20.402  29.978  1.00 25.08      O
ATOM  1433  N   HIS A 206     31.126  21.024  31.004  1.00 25.00      N
ATOM  1434  CA  HIS A 206     30.389  19.861  30.507  1.00 25.50      C
ATOM  1435  CB  HIS A 206     29.096  19.644  31.301  1.00 25.48      C
ATOM  1436  CG  HIS A 206     29.243  18.752  32.496  1.00 25.77      C
ATOM  1437  CD2 HIS A 206     28.818  17.485  32.715  1.00 26.12      C
ATOM  1438  ND1 HIS A 206     29.853  19.158  33.664  1.00 26.12      N
ATOM  1439  CE1 HIS A 206     29.794  18.182  34.552  1.00 26.27      C
ATOM  1440  NE2 HIS A 206     29.171  17.156  34.001  1.00 25.97      N
ATOM  1441  C   HIS A 206     29.990  20.056  29.038  1.00 25.23      C
ATOM  1442  O   HIS A 206     29.915  19.096  28.261  1.00 24.85      O
ATOM  1443  N   PHE A 207     29.739  21.305  28.661  1.00 25.12      N
ATOM  1444  CA  PHE A 207     29.259  21.602  27.314  1.00 24.78      C
ATOM  1445  CB  PHE A 207     28.765  23.059  27.262  1.00 24.50      C
ATOM  1446  CG  PHE A 207     27.625  23.346  28.223  1.00 24.94      C
ATOM  1447  CD1 PHE A 207     27.171  24.651  28.422  1.00 24.92      C
ATOM  1448  CD2 PHE A 207     27.019  22.311  28.945  1.00 25.02      C
ATOM  1449  CE1 PHE A 207     26.137  24.924  29.322  1.00 24.91      C
ATOM  1450  CE2 PHE A 207     25.984  22.574  29.848  1.00 24.68      C
ATOM  1451  CZ  PHE A 207     25.544  23.881  30.037  1.00 24.50      C
ATOM  1452  C   PHE A 207     30.139  21.263  26.117  1.00 24.23      C
ATOM  1453  O   PHE A 207     29.624  20.794  25.105  1.00 24.49      O
ATOM  1454  N   PRO A 208     31.467  21.485  26.199  1.00 24.05      N
ATOM  1455  CD  PRO A 208     32.268  22.196  27.216  1.00 23.52      C
ATOM  1456  CA  PRO A 208     32.292  21.140  25.035  1.00 23.79      C
ATOM  1457  CB  PRO A 208     33.709  21.443  25.519  1.00 23.37      C
ATOM  1458  CG  PRO A 208     33.497  22.617  26.415  1.00 23.62      C
ATOM  1459  C   PRO A 208     32.111  19.665  24.650  1.00 23.75      C
ATOM  1460  O   PRO A 208     32.307  19.283  23.496  1.00 23.71      O
ATOM  1461  N   LEU A 209     31.731  18.846  25.628  1.00 24.35      N
ATOM  1462  CA  LEU A 209     31.510  17.416  25.400  1.00 24.73      C
ATOM  1463  CB  LEU A 209     31.225  16.703  26.730  1.00 24.44      C
ATOM  1464  CG  LEU A 209     32.351  16.705  27.763  1.00 24.17      C
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Figure 10AA

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ATOM  1465  CD1 LEU A 209     31.856  16.084  29.055  1.00 24.39      C
ATOM  1466  CD2 LEU A 209     33.546  15.940  27.213  1.00 25.04      C
ATOM  1467  C   LEU A 209     30.330  17.193  24.453  1.00 24.96      C
ATOM  1468  O   LEU A 209     30.185  16.115  23.871  1.00 25.40      O
ATOM  1469  N   LEU A 210     29.492  18.214  24.311  1.00 25.40      N
ATOM  1470  CA  LEU A 210     28.313  18.150  23.445  1.00 26.09      C
ATOM  1471  CB  LEU A 210     27.091  18.700  24.187  1.00 26.08      C
ATOM  1472  CG  LEU A 210     26.612  17.931  25.424  1.00 26.43      C
ATOM  1473  CD1 LEU A 210     25.590  18.754  26.165  1.00 26.49      C
ATOM  1474  CD2 LEU A 210     26.031  16.587  25.006  1.00 26.75      C
ATOM  1475  C   LEU A 210     28.513  18.956  22.165  1.00 26.97      C
ATOM  1476  O   LEU A 210     27.551  19.238  21.443  1.00 26.49      O
ATOM  1477  N   GLN A 211     29.754  19.325  21.877  1.00 27.84      N
ATOM  1478  CA  GLN A 211     30.018  20.125  20.689  1.00 29.76      C
ATOM  1479  CB  GLN A 211     31.525  20.241  20.426  1.00 31.43      C
ATOM  1480  CG  GLN A 211     31.822  21.058  19.169  1.00 35.04      C
ATOM  1481  CD  GLN A 211     33.278  21.444  19.027  1.00 36.79      C
ATOM  1482  OE1 GLN A 211     33.814  22.205  19.840  1.00 38.21      O
ATOM  1483  NE2 GLN A 211     33.929  20.926  17.985  1.00 37.92      N
ATOM  1484  C   GLN A 211     29.319  19.624  19.428  1.00 29.78      C
ATOM  1485  O   GLN A 211     28.629  20.390  18.757  1.00 29.75      O
ATOM  1486  N   GLU A 212     29.482  18.346  19.104  1.00 30.23      N
ATOM  1487  CA  GLU A 212     28.857  17.805  17.898  1.00 31.41      C
ATOM  1488  CB  GLU A 212     29.173  16.312  17.750  1.00 33.48      C
ATOM  1489  CG  GLU A 212     28.789  15.739  16.391  1.00 36.83      C
ATOM  1490  CD  GLU A 212     29.709  14.609  15.940  1.00 38.98      C
ATOM  1491  OE1 GLU A 212     30.921  14.860  15.738  1.00 40.36      O
ATOM  1492  OE2 GLU A 212     29.223  13.468  15.786  1.00 40.67      O
ATOM  1493  C   GLU A 212     27.348  18.023  17.894  1.00 30.99      C
ATOM  1494  O   GLU A 212     26.791  18.548  16.928  1.00 30.68      O
ATOM  1495  N   GLU A 213     26.692  17.628  18.983  1.00 30.23      N
ATOM  1496  CA  GLU A 213     25.253  17.788  19.103  1.00 29.95      C
ATOM  1497  CB  GLU A 213     24.760  17.214  20.436  1.00 30.26      C
ATOM  1498  CG  GLU A 213     24.844  15.697  20.570  1.00 31.58      C
ATOM  1499  CD  GLU A 213     26.237  15.179  20.909  1.00 32.64      C
ATOM  1500  OE1 GLU A 213     27.150  15.992  21.177  1.00 32.86      O
ATOM  1501  OE2 GLU A 213     26.412  13.942  20.915  1.00 33.12      O
ATOM  1502  C   GLU A 213     24.840  19.258  19.005  1.00 29.41      C
ATOM  1503  O   GLU A 213     23.857  19.587  18.338  1.00 29.01      O
ATOM  1504  N   LEU A 214     25.580  20.137  19.681  1.00 28.84      N
ATOM  1505  CA  LEU A 214     25.268  21.567  19.656  1.00 28.43      C
ATOM  1506  CB  LEU A 214     26.216  22.348  20.570  1.00 28.13      C
ATOM  1507  CG  LEU A 214     25.977  22.173  22.075  1.00 27.63      C
ATOM  1508  CD1 LEU A 214     27.109  22.818  22.862  1.00 27.49      C
ATOM  1509  CD2 LEU A 214     24.626  22.791  22.447  1.00 27.85      C
ATOM  1510  C   LEU A 214     25.348  22.136  18.247  1.00 28.83      C
ATOM  1511  O   LEU A 214     24.507  22.937  17.845  1.00 27.87      O
ATOM  1512  N   LEU A 215     26.356  21.713  17.498  1.00 29.30      N
ATOM  1513  CA  LEU A 215     26.528  22.202  16.142  1.00 30.96      C
ATOM  1514  CB  LEU A 215     27.918  21.822  15.630  1.00 30.54      C
ATOM  1515  CG  LEU A 215     29.025  22.593  16.358  1.00 30.81      C
ATOM  1516  CD1 LEU A 215     30.386  22.124  15.895  1.00 30.80      C
ATOM  1517  CD2 LEU A 215     28.858  24.084  16.093  1.00 30.46      C
ATOM  1518  C   LEU A 215     25.440  21.709  15.191  1.00 31.93      C
ATOM  1519  O   LEU A 215     25.211  22.308  14.145  1.00 32.43      O
ATOM  1520  N   GLN A 216     24.762  20.625  15.551  1.00 33.13      N
ATOM  1521  CA  GLN A 216     23.695  20.108  14.701  1.00 34.56      C
ATOM  1522  CB  GLN A 216     23.435  18.625  14.988  1.00 35.66      C
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Figure 10BB

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ATOM  1523  CG  GLN A 216      24.610  17.700  14.728  1.00 37.89           C
ATOM  1524  CD  GLN A 216      24.241  16.238  14.906  1.00 39.33           C
ATOM  1525  OE1 GLN A 216      23.524  15.665  14.083  1.00 41.09           O
ATOM  1526  NE2 GLN A 216      24.717  15.629  15.988  1.00 39.66           N
ATOM  1527  C   GLN A 216      22.406  20.888  14.939  1.00 34.80           C
ATOM  1528  O   GLN A 216      21.569  21.014  14.047  1.00 35.06           O
ATOM  1529  N   VAL A 217      22.258  21.416  16.148  1.00 34.71           N
ATOM  1530  CA  VAL A 217      21.064  22.156  16.531  1.00 35.07           C
ATOM  1531  CB  VAL A 217      20.710  21.866  18.016  1.00 35.06           C
ATOM  1532  CG1 VAL A 217      19.504  22.685  18.451  1.00 35.49           C
ATOM  1533  CG2 VAL A 217      20.435  20.390  18.192  1.00 35.11           C
ATOM  1534  C   VAL A 217      21.164  23.664  16.336  1.00 35.24           C
ATOM  1535  O   VAL A 217      20.199  24.304  15.925  1.00 34.92           O
ATOM  1536  N   LEU A 218      22.326  24.233  16.640  1.00 35.48           N
ATOM  1537  CA  LEU A 218      22.520  25.674  16.511  1.00 35.98           C
ATOM  1538  CB  LEU A 218      23.837  26.097  17.175  1.00 35.20           C
ATOM  1539  CG  LEU A 218      23.954  25.958  18.699  1.00 34.74           C
ATOM  1540  CD1 LEU A 218      25.415  26.086  19.099  1.00 33.85           C
ATOM  1541  CD2 LEU A 218      23.107  27.018  19.395  1.00 34.29           C
ATOM  1542  C   LEU A 218      22.520  26.143  15.059  1.00 36.85           C
ATOM  1543  O   LEU A 218      22.923  25.408  14.154  1.00 36.56           O
ATOM  1544  N   PRO A 219      22.062  27.382  14.819  1.00 37.78           N
ATOM  1545  CD  PRO A 219      21.542  28.360  15.788  1.00 38.25           C
ATOM  1546  CA  PRO A 219      22.026  27.929  13.461  1.00 38.69           C
ATOM  1547  CB  PRO A 219      21.507  29.354  13.664  1.00 38.57           C
ATOM  1548  CG  PRO A 219      21.840  29.660  15.088  1.00 38.75           C
ATOM  1549  C   PRO A 219      23.390  27.895  12.785  1.00 39.23           C
ATOM  1550  O   PRO A 219      24.422  28.136  13.419  1.00 39.41           O
ATOM  1551  N   GLU A 220      23.381  27.591  11.494  1.00 39.72           N
ATOM  1552  CA  GLU A 220      24.600  27.502  10.698  1.00 40.27           C
ATOM  1553  CB  GLU A 220      24.250  27.481   9.207  1.00 41.80           C
ATOM  1554  CG  GLU A 220      22.941  26.777   8.874  1.00 43.87           C
ATOM  1555  CD  GLU A 220      22.413  27.165   7.498  1.00 45.18           C
ATOM  1556  OE1 GLU A 220      23.087  26.854   6.492  1.00 45.89           O
ATOM  1557  OE2 GLU A 220      21.325  27.789   7.425  1.00 45.96           O
ATOM  1558  C   GLU A 220      25.505  28.698  10.972  1.00 39.71           C
ATOM  1559  O   GLU A 220      25.023  29.808  11.211  1.00 40.05           O
ATOM  1560  N   GLY A 221      26.813  28.466  10.946  1.00 38.99           N
ATOM  1561  CA  GLY A 221      27.758  29.547  11.162  1.00 38.23           C
ATOM  1562  C   GLY A 221      28.059  29.947  12.595  1.00 37.79           C
ATOM  1563  O   GLY A 221      28.875  30.842  12.818  1.00 37.76           O
ATOM  1564  N   THR A 222      27.414  29.308  13.566  1.00 36.92           N
ATOM  1565  CA  THR A 222      27.669  29.637  14.967  1.00 36.06           C
ATOM  1566  CB  THR A 222      26.600  29.039  15.911  1.00 36.28           C
ATOM  1567  OG1 THR A 222      25.286  29.441  15.489  1.00 35.84           O
ATOM  1568  CG2 THR A 222      26.836  29.530  17.331  1.00 35.92           C
ATOM  1569  C   THR A 222      29.031  29.082  15.375  1.00 35.26           C
ATOM  1570  O   THR A 222      29.325  27.904  15.159  1.00 35.42           O
ATOM  1571  N   ARG A 223      29.864  29.934  15.962  1.00 33.89           N
ATOM  1572  CA  ARG A 223      31.187  29.515  16.395  1.00 32.73           C
ATOM  1573  CB  ARG A 223      32.213  30.593  16.048  1.00 33.48           C
ATOM  1574  CG  ARG A 223      33.634  30.257  16.448  1.00 34.74           C
ATOM  1575  CD  ARG A 223      34.572  31.304  15.885  1.00 35.80           C
ATOM  1576  NE  ARG A 223      35.976  31.038  16.180  1.00 36.83           N
ATOM  1577  CZ  ARG A 223      36.975  31.735  15.653  1.00 36.90           C
ATOM  1578  NH1 ARG A 223      36.709  32.722  14.808  1.00 37.42           N
ATOM  1579  NH2 ARG A 223      38.229  31.460  15.974  1.00 37.62           N
ATOM  1580  C   ARG A 223      31.204  29.254  17.896  1.00 31.22           C
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Figure 10CC

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ATOM  1581  O   ARG A 223     30.823  30.118  18.684  1.00 31.14           O
ATOM  1582  N   LEU A 224     31.649  28.063  18.287  1.00 29.77           N
ATOM  1583  CA  LEU A 224     31.714  27.702  19.698  1.00 28.63           C
ATOM  1584  CB  LEU A 224     31.501  26.196  19.885  1.00 28.14           C
ATOM  1585  CG  LEU A 224     30.191  25.617  19.343  1.00 28.31           C
ATOM  1586  CD1 LEU A 224     30.145  24.122  19.618  1.00 27.77           C
ATOM  1587  CD2 LEU A 224     29.011  26.321  19.990  1.00 28.16           C
ATOM  1588  C   LEU A 224     33.074  28.088  20.267  1.00 28.22           C
ATOM  1589  O   LEU A 224     34.113  27.855  19.646  1.00 27.72           O
ATOM  1590  N   VAL A 225     33.055  28.678  21.452  1.00 27.59           N
ATOM  1591  CA  VAL A 225     34.279  29.094  22.114  1.00 27.22           C
ATOM  1592  CB  VAL A 225     34.386  30.638  22.165  1.00 27.19           C
ATOM  1593  CG1 VAL A 225     35.669  31.047  22.875  1.00 27.27           C
ATOM  1594  CG2 VAL A 225     34.346  31.219  20.755  1.00 27.27           C
ATOM  1595  C   VAL A 225     34.315  28.573  23.553  1.00 27.00           C
ATOM  1596  O   VAL A 225     33.343  28.707  24.291  1.00 26.02           O
ATOM  1597  N   ASP A 226     35.427  27.965  23.946  1.00 27.26           N
ATOM  1598  CA  ASP A 226     35.555  27.505  25.319  1.00 28.37           C
ATOM  1599  CB  ASP A 226     35.210  26.008  25.469  1.00 29.27           C
ATOM  1600  CG  ASP A 226     36.130  25.095  24.689  1.00 30.58           C
ATOM  1601  OD1 ASP A 226     37.361  25.166  24.874  1.00 31.43           O
ATOM  1602  OD2 ASP A 226     35.613  24.283  23.891  1.00 32.27           O
ATOM  1603  C   ASP A 226     36.952  27.818  25.835  1.00 28.68           C
ATOM  1604  O   ASP A 226     37.767  28.418  25.126  1.00 28.29           O
ATOM  1605  N   SER A 227     37.222  27.409  27.067  1.00 29.15           N
ATOM  1606  CA  SER A 227     38.493  27.693  27.730  1.00 30.16           C
ATOM  1607  CB  SER A 227     38.212  28.003  29.200  1.00 30.84           C
ATOM  1608  OG  SER A 227     37.330  29.105  29.315  1.00 33.08           O
ATOM  1609  C   SER A 227     39.568  26.613  27.662  1.00 29.90           C
ATOM  1610  O   SER A 227     40.696  26.833  28.118  1.00 30.24           O
ATOM  1611  N   GLY A 228     39.221  25.467  27.089  1.00 29.54           N
ATOM  1612  CA  GLY A 228     40.133  24.333  27.004  1.00 29.07           C
ATOM  1613  C   GLY A 228     41.586  24.537  26.605  1.00 29.10           C
ATOM  1614  O   GLY A 228     42.494  24.267  27.400  1.00 28.05           O
ATOM  1615  N   ALA A 229     41.810  24.983  25.368  1.00 28.66           N
ATOM  1616  CA  ALA A 229     43.161  25.208  24.868  1.00 28.46           C
ATOM  1617  CB  ALA A 229     43.113  25.634  23.399  1.00 28.89           C
ATOM  1618  C   ALA A 229     43.900  26.257  25.694  1.00 28.23           C
ATOM  1619  O   ALA A 229     45.095  26.127  25.934  1.00 28.75           O
ATOM  1620  N   ALA A 230     43.191  27.290  26.135  1.00 28.21           N
ATOM  1621  CA  ALA A 230     43.820  28.341  26.937  1.00 28.47           C
ATOM  1622  CB  ALA A 230     42.872  29.512  27.106  1.00 28.62           C
ATOM  1623  C   ALA A 230     44.248  27.821  28.309  1.00 29.04           C
ATOM  1624  O   ALA A 230     45.253  28.281  28.871  1.00 28.26           O
ATOM  1625  N   ILE A 231     43.476  26.874  28.850  1.00 28.95           N
ATOM  1626  CA  ILE A 231     43.785  26.281  30.149  1.00 29.12           C
ATOM  1627  CB  ILE A 231     42.651  25.351  30.636  1.00 29.08           C
ATOM  1628  CG2 ILE A 231     43.053  24.671  31.953  1.00 28.24           C
ATOM  1629  CG1 ILE A 231     41.364  26.152  30.804  1.00 29.21           C
ATOM  1630  CD1 ILE A 231     41.467  27.238  31.820  1.00 28.47           C
ATOM  1631  C   ILE A 231     45.035  25.442  29.986  1.00 29.33           C
ATOM  1632  O   ILE A 231     45.915  25.428  30.850  1.00 29.46           O
ATOM  1633  N   ALA A 232     45.097  24.729  28.870  1.00 29.68           N
ATOM  1634  CA  ALA A 232     46.237  23.884  28.566  1.00 30.26           C
ATOM  1635  CB  ALA A 232     46.030  23.206  27.223  1.00 30.00           C
ATOM  1636  C   ALA A 232     47.493  24.764  28.538  1.00 31.19           C
ATOM  1637  O   ALA A 232     48.487  24.458  29.202  1.00 31.16           O
ATOM  1638  N   ARG A 233     47.437  25.863  27.784  1.00 31.62           N
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Figure 10DD

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ATOM  1639 CA  ARG A 233     48.576  26.776  27.695  1.00 32.55      C
ATOM  1640 CB  ARG A 233     48.273  27.932  26.729  1.00 32.86      C
ATOM  1641 CG  ARG A 233     48.187  27.516  25.259  1.00 32.98      C
ATOM  1642 CD  ARG A 233     48.181  28.745  24.352  1.00 34.06      C
ATOM  1643 NE  ARG A 233     46.982  29.563  24.530  1.00 34.89      N
ATOM  1644 CZ  ARG A 233     45.818  29.316  23.934  1.00 35.40      C
ATOM  1645 NH1 ARG A 233     45.697  28.281  23.115  1.00 35.59      N
ATOM  1646 NH2 ARG A 233     44.770  30.094  24.168  1.00 35.89      N
ATOM  1647 C   ARG A 233     48.952  27.332  29.069  1.00 32.57      C
ATOM  1648 O   ARG A 233     50.129  27.422  29.402  1.00 32.69      O
ATOM  1649 N   ARG A 234     47.957  27.702  29.869  1.00 32.61      N
ATOM  1650 CA  ARG A 234     48.229  28.229  31.206  1.00 32.84      C
ATOM  1651 CB  ARG A 234     46.934  28.713  31.861  1.00 32.78      C
ATOM  1652 CG  ARG A 234     47.107  29.235  33.280  1.00 33.27      C
ATOM  1653 CD  ARG A 234     48.098  30.400  33.357  1.00 33.63      C
ATOM  1654 NE  ARG A 234     48.091  31.010  34.685  1.00 34.67      N
ATOM  1655 CZ  ARG A 234     48.883  32.009  35.060  1.00 34.84      C
ATOM  1656 NH1 ARG A 234     49.759  32.519  34.204  1.00 35.01      N
ATOM  1657 NH2 ARG A 234     48.794  32.502  36.289  1.00 35.15      N
ATOM  1658 C   ARG A 234     48.885  27.155  32.082  1.00 33.23      C
ATOM  1659 O   ARG A 234     49.760  27.458  32.901  1.00 33.10      O
ATOM  1660 N   THR A 235     48.464  25.906  31.897  1.00 32.93      N
ATOM  1661 CA  THR A 235     49.007  24.778  32.652  1.00 33.19      C
ATOM  1662 CB  THR A 235     48.201  23.486  32.368  1.00 32.74      C
ATOM  1663 OG1 THR A 235     46.879  23.637  32.899  1.00 32.01      O
ATOM  1664 CG2 THR A 235     48.867  22.262  33.013  1.00 32.30      C
ATOM  1665 C   THR A 235     50.475  24.564  32.290  1.00 33.74      C
ATOM  1666 O   THR A 235     51.327  24.396  33.170  1.00 33.08      O
ATOM  1667 N   ALA A 236     50.767  24.586  30.993  1.00 34.60      N
ATOM  1668 CA  ALA A 236     52.135  24.415  30.519  1.00 35.65      C
ATOM  1669 CB  ALA A 236     52.163  24.387  28.994  1.00 35.86      C
ATOM  1670 C   ALA A 236     53.021  25.548  31.042  1.00 36.35      C
ATOM  1671 O   ALA A 236     54.180  25.328  31.388  1.00 36.64      O
ATOM  1672 N   TRP A 237     52.480  26.761  31.109  1.00 37.16      N
ATOM  1673 CA  TRP A 237     53.261  27.893  31.599  1.00 38.00      C
ATOM  1674 CB  TRP A 237     52.509  29.208  31.380  1.00 38.98      C
ATOM  1675 CG  TRP A 237     53.355  30.429  31.649  1.00 40.50      C
ATOM  1676 CD2 TRP A 237     53.400  31.199  32.859  1.00 40.98      C
ATOM  1677 CE2 TRP A 237     54.352  32.228  32.667  1.00 41.43      C
ATOM  1678 CE3 TRP A 237     52.730  31.120  34.087  1.00 41.27      C
ATOM  1679 CD1 TRP A 237     54.260  31.006  30.797  1.00 41.31      C
ATOM  1680 NE1 TRP A 237     54.861  32.088  31.402  1.00 41.47      N
ATOM  1681 CZ2 TRP A 237     54.650  33.171  33.659  1.00 41.56      C
ATOM  1682 CZ3 TRP A 237     53.028  32.058  35.075  1.00 41.51      C
ATOM  1683 CH2 TRP A 237     53.980  33.070  34.852  1.00 41.65      C
ATOM  1684 C   TRP A 237     53.573  27.744  33.092  1.00 38.01      C
ATOM  1685 O   TRP A 237     54.687  28.035  33.537  1.00 37.78      O
ATOM  1686 N   LEU A 238     52.585  27.299  33.862  1.00 37.56      N
ATOM  1687 CA  LEU A 238     52.762  27.127  35.299  1.00 37.57      C
ATOM  1688 CB  LEU A 238     51.408  26.902  35.975  1.00 36.67      C
ATOM  1689 CG  LEU A 238     50.478  28.114  35.957  1.00 36.43      C
ATOM  1690 CD1 LEU A 238     49.116  27.731  36.487  1.00 36.24      C
ATOM  1691 CD2 LEU A 238     51.077  29.235  36.794  1.00 36.56      C
ATOM  1692 C   LEU A 238     53.703  25.977  35.622  1.00 37.81      C
ATOM  1693 O   LEU A 238     54.461  26.040  36.591  1.00 37.91      O
ATOM  1694 N   LEU A 239     53.660  24.923  34.819  1.00 38.48      N
ATOM  1695 CA  LEU A 239     54.540  23.791  35.057  1.00 39.58      C
ATOM  1696 CB  LEU A 239     54.163  22.619  34.149  1.00 39.09      C
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Figure 10EE

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ATOM  1697  CG  LEU A 239      52.839  21.921  34.493  1.00 38.87      C
ATOM  1698  CD1 LEU A 239      52.520  20.870  33.447  1.00 38.45      C
ATOM  1699  CD2 LEU A 239      52.936  21.293  35.881  1.00 38.47      C
ATOM  1700  C   LEU A 239      55.979  24.224  34.791  1.00 40.79      C
ATOM  1701  O   LEU A 239      56.927  23.586  35.249  1.00 40.92      O
ATOM  1702  N   GLU A 240      56.129  25.324  34.060  1.00 41.65      N
ATOM  1703  CA  GLU A 240      57.448  25.837  33.719  1.00 42.84      C
ATOM  1704  CB  GLU A 240      57.444  26.409  32.297  1.00 43.65      C
ATOM  1705  CG  GLU A 240      57.275  25.369  31.200  1.00 45.38      C
ATOM  1706  CD  GLU A 240      58.319  24.268  31.280  1.00 46.58      C
ATOM  1707  OE1 GLU A 240      59.529  24.596  31.325  1.00 47.04      O
ATOM  1708  OE2 GLU A 240      57.929  23.076  31.296  1.00 47.22      O
ATOM  1709  C   GLU A 240      57.961  26.905  34.667  1.00 43.09      C
ATOM  1710  O   GLU A 240      59.150  26.944  34.968  1.00 43.08      O
ATOM  1711  N   HIS A 241      57.069  27.767  35.143  1.00 43.49      N
ATOM  1712  CA  HIS A 241      57.486  28.858  36.011  1.00 44.38      C
ATOM  1713  CB  HIS A 241      57.070  30.186  35.364  1.00 45.65      C
ATOM  1714  CG  HIS A 241      57.586  30.367  33.967  1.00 47.27      C
ATOM  1715  CD2 HIS A 241      58.415  29.604  33.215  1.00 47.86      C
ATOM  1716  ND1 HIS A 241      57.237  31.442  33.178  1.00 47.83      N
ATOM  1717  CE1 HIS A 241      57.825  31.332  32.000  1.00 48.31      C
ATOM  1718  NE2 HIS A 241      58.546  30.225  31.996  1.00 48.70      N
ATOM  1719  C   HIS A 241      57.024  28.846  37.473  1.00 44.07      C
ATOM  1720  O   HIS A 241      57.400  29.741  38.232  1.00 44.13      O
ATOM  1721  N   GLU A 242      56.236  27.853  37.886  1.00 43.53      N
ATOM  1722  CA  GLU A 242      55.754  27.839  39.269  1.00 42.98      C
ATOM  1723  CB  GLU A 242      54.421  28.589  39.359  1.00 43.70      C
ATOM  1724  CG  GLU A 242      54.522  30.087  39.173  1.00 44.78      C
ATOM  1725  CD  GLU A 242      53.167  30.759  39.210  1.00 45.69      C
ATOM  1726  OE1 GLU A 242      52.341  30.397  40.081  1.00 45.73      O
ATOM  1727  OE2 GLU A 242      52.930  31.658  38.375  1.00 46.45      O
ATOM  1728  C   GLU A 242      55.578  26.498  39.977  1.00 42.31      C
ATOM  1729  O   GLU A 242      55.680  26.430  41.200  1.00 42.11      O
ATOM  1730  N   ALA A 243      55.306  25.439  39.224  1.00 41.35      N
ATOM  1731  CA  ALA A 243      55.072  24.127  39.820  1.00 40.63      C
ATOM  1732  CB  ALA A 243      54.557  23.163  38.758  1.00 40.62      C
ATOM  1733  C   ALA A 243      56.262  23.498  40.540  1.00 40.38      C
ATOM  1734  O   ALA A 243      57.382  23.480  40.025  1.00 39.78      O
ATOM  1735  N   PRO A 244      56.028  22.970  41.753  1.00 39.91      N
ATOM  1736  CD  PRO A 244      54.781  23.031  42.540  1.00 39.77      C
ATOM  1737  CA  PRO A 244      57.102  22.331  42.518  1.00 39.80      C
ATOM  1738  CB  PRO A 244      56.495  22.194  43.914  1.00 39.91      C
ATOM  1739  CG  PRO A 244      55.026  21.998  43.617  1.00 39.75      C
ATOM  1740  C   PRO A 244      57.415  20.982  41.875  1.00 39.90      C
ATOM  1741  O   PRO A 244      56.603  20.452  41.114  1.00 39.34      O
ATOM  1742  N   ASP A 245      58.588  20.431  42.176  1.00 40.00      N
ATOM  1743  CA  ASP A 245      59.011  19.149  41.615  1.00 40.24      C
ATOM  1744  CB  ASP A 245      60.516  18.947  41.853  1.00 41.09      C
ATOM  1745  CG  ASP A 245      61.071  17.750  41.102  1.00 41.84      C
ATOM  1746  OD1 ASP A 245      62.133  17.226  41.501  1.00 42.48      O
ATOM  1747  OD2 ASP A 245      60.455  17.334  40.100  1.00 42.69      O
ATOM  1748  C   ASP A 245      58.245  17.957  42.193  1.00 40.06      C
ATOM  1749  O   ASP A 245      58.817  17.131  42.907  1.00 40.25      O
ATOM  1750  N   ALA A 246      56.954  17.864  41.882  1.00 39.77      N
ATOM  1751  CA  ALA A 246      56.121  16.765  42.364  1.00 39.54      C
ATOM  1752  CB  ALA A 246      54.836  17.313  42.982  1.00 39.39      C
ATOM  1753  C   ALA A 246      55.796  15.857  41.182  1.00 39.56      C
ATOM  1754  O   ALA A 246      54.964  16.194  40.338  1.00 39.19      O
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Figure 10FF

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ATOM  1755 N   LYS A 247     56.446  14.699  41.129  1.00 39.47      N
ATOM  1756 CA  LYS A 247     56.245  13.771  40.024  1.00 39.58      C
ATOM  1757 CB  LYS A 247     57.416  13.892  39.049  1.00 40.22      C
ATOM  1758 CG  LYS A 247     58.777  13.707  39.705  1.00 41.70      C
ATOM  1759 CD  LYS A 247     59.910  13.916  38.706  1.00 43.00      C
ATOM  1760 CE  LYS A 247     61.266  13.866  39.394  1.00 43.78      C
ATOM  1761 NZ  LYS A 247     61.482  12.561  40.080  1.00 45.10      N
ATOM  1762 C   LYS A 247     56.097  12.317  40.450  1.00 39.34      C
ATOM  1763 O   LYS A 247     56.453  11.941  41.564  1.00 39.51      O
ATOM  1764 N   SER A 248     55.583  11.499  39.539  1.00 38.98      N
ATOM  1765 CA  SER A 248     55.385  10.082  39.793  1.00 38.69      C
ATOM  1766 CB  SER A 248     54.009   9.856  40.435  1.00 38.62      C
ATOM  1767 OG  SER A 248     53.728   8.479  40.587  1.00 38.23      O
ATOM  1768 C   SER A 248     55.487   9.286  38.492  1.00 38.63      C
ATOM  1769 O   SER A 248     55.262   9.820  37.405  1.00 38.34      O
ATOM  1770 N   ALA A 249     55.830   8.007  38.609  1.00 38.50      N
ATOM  1771 CA  ALA A 249     55.941   7.150  37.438  1.00 38.58      C
ATOM  1772 CB  ALA A 249     57.195   6.275  37.536  1.00 38.58      C
ATOM  1773 C   ALA A 249     54.691   6.281  37.308  1.00 38.38      C
ATOM  1774 O   ALA A 249     54.529   5.558  36.326  1.00 38.36      O
ATOM  1775 N   ASP A 250     53.805   6.357  38.299  1.00 38.17      N
ATOM  1776 CA  ASP A 250     52.572   5.576  38.269  1.00 37.75      C
ATOM  1777 CB  ASP A 250     51.765   5.767  39.562  1.00 38.49      C
ATOM  1778 CG  ASP A 250     52.435   5.136  40.773  1.00 39.62      C
ATOM  1779 OD1 ASP A 250     53.432   4.403  40.593  1.00 40.12      O
ATOM  1780 OD2 ASP A 250     51.960   5.365  41.909  1.00 39.88      O
ATOM  1781 C   ASP A 250     51.722   5.995  37.076  1.00 36.87      C
ATOM  1782 O   ASP A 250     51.859   7.106  36.563  1.00 37.25      O
ATOM  1783 N   ALA A 251     50.845   5.100  36.636  1.00 36.01      N
ATOM  1784 CA  ALA A 251     49.971   5.379  35.504  1.00 34.97      C
ATOM  1785 CB  ALA A 251     49.359   4.086  34.990  1.00 35.52      C
ATOM  1786 C   ALA A 251     48.868   6.349  35.918  1.00 33.97      C
ATOM  1787 O   ALA A 251     48.624   6.547  37.107  1.00 33.63      O
ATOM  1788 N   ASN A 252     48.206   6.948  34.933  1.00 32.74      N
ATOM  1789 CA  ASN A 252     47.131   7.894  35.204  1.00 31.53      C
ATOM  1790 CB  ASN A 252     46.550   8.451  33.903  1.00 31.29      C
ATOM  1791 CG  ASN A 252     47.583   9.156  33.059  1.00 31.11      C
ATOM  1792 OD1 ASN A 252     48.532   9.745  33.580  1.00 30.92      O
ATOM  1793 ND2 ASN A 252     47.397   9.118  31.747  1.00 31.17      N
ATOM  1794 C   ASN A 252     46.025   7.202  35.983  1.00 30.57      C
ATOM  1795 O   ASN A 252     45.737   6.032  35.755  1.00 30.37      O
ATOM  1796 N   ILE A 253     45.398   7.929  36.896  1.00 29.76      N
ATOM  1797 CA  ILE A 253     44.331   7.340  37.694  1.00 29.03      C
ATOM  1798 CB  ILE A 253     44.880   6.919  39.080  1.00 29.45      C
ATOM  1799 CG2 ILE A 253     45.374   8.139  39.833  1.00 29.70      C
ATOM  1800 CG1 ILE A 253     43.802   6.198  39.888  1.00 30.29      C
ATOM  1801 CD1 ILE A 253     44.292   5.736  41.244  1.00 31.33      C
ATOM  1802 C   ILE A 253     43.141   8.286  37.875  1.00 28.11      C
ATOM  1803 O   ILE A 253     43.297   9.512  37.893  1.00 27.59      O
ATOM  1804 N   ALA A 254     41.948   7.705  37.979  1.00 26.97      N
ATOM  1805 CA  ALA A 254     40.733   8.479  38.183  1.00 25.96      C
ATOM  1806 CB  ALA A 254     39.685   8.123  37.125  1.00 25.54      C
ATOM  1807 C   ALA A 254     40.200   8.167  39.578  1.00 25.64      C
ATOM  1808 O   ALA A 254     40.217   7.010  40.013  1.00 25.40      O
ATOM  1809 N   PHE A 255     39.749   9.203  40.276  1.00 24.93      N
ATOM  1810 CA  PHE A 255     39.188   9.061  41.619  1.00 25.25      C
ATOM  1811 CB  PHE A 255     39.931   9.936  42.633  1.00 24.82      C
ATOM  1812 CG  PHE A 255     41.278   9.416  43.044  1.00 25.59      C
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Figure 10GG

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ATOM  1813 CD1 PHE A 255     42.399  10.235  42.953  1.00 25.46      C
ATOM  1814 CD2 PHE A 255     41.422   8.132  43.559  1.00 26.01      C
ATOM  1815 CE1 PHE A 255     43.650   9.789  43.368  1.00 26.29      C
ATOM  1816 CE2 PHE A 255     42.671   7.668  43.982  1.00 26.91      C
ATOM  1817 CZ  PHE A 255     43.790   8.500  43.884  1.00 26.72      C
ATOM  1818 C   PHE A 255     37.726   9.503  41.663  1.00 25.33      C
ATOM  1819 O   PHE A 255     37.370  10.562  41.140  1.00 25.42      O
ATOM  1820 N   CYS A 256     36.874   8.698  42.284  1.00 25.82      N
ATOM  1821 CA  CYS A 256     35.482   9.099  42.462  1.00 26.46      C
ATOM  1822 CB  CYS A 256     34.512   8.041  41.920  1.00 27.23      C
ATOM  1823 SG  CYS A 256     34.653   6.407  42.664  1.00 29.02      S
ATOM  1824 C   CYS A 256     35.364   9.237  43.983  1.00 26.79      C
ATOM  1825 O   CYS A 256     36.246   8.775  44.715  1.00 26.33      O
ATOM  1826 N   MET A 257     34.308   9.877  44.475  1.00 27.23      N
ATOM  1827 CA  MET A 257     34.174  10.030  45.924  1.00 27.99      C
ATOM  1828 CB  MET A 257     33.566  11.395  46.270  1.00 28.01      C
ATOM  1829 CG  MET A 257     34.365  12.586  45.730  1.00 28.41      C
ATOM  1830 SD  MET A 257     36.165  12.503  46.030  1.00 29.78      S
ATOM  1831 CE  MET A 257     36.802  12.840  44.372  1.00 29.70      C
ATOM  1832 C   MET A 257     33.343   8.903  46.536  1.00 28.39      C
ATOM  1833 O   MET A 257     33.310   8.733  47.754  1.00 28.39      O
ATOM  1834 N   ALA A 258     32.691   8.128  45.679  1.00 29.08      N
ATOM  1835 CA  ALA A 258     31.880   6.999  46.117  1.00 30.02      C
ATOM  1836 CB  ALA A 258     30.474   7.460  46.494  1.00 29.75      C
ATOM  1837 C   ALA A 258     31.814   6.007  44.969  1.00 30.76      C
ATOM  1838 O   ALA A 258     31.509   6.379  43.837  1.00 30.44      O
ATOM  1839 N   MET A 259     32.111   4.747  45.259  1.00 31.73      N
ATOM  1840 CA  MET A 259     32.084   3.712  44.236  1.00 32.90      C
ATOM  1841 CB  MET A 259     32.945   2.527  44.675  1.00 34.30      C
ATOM  1842 CG  MET A 259     33.303   1.566  43.559  1.00 36.54      C
ATOM  1843 SD  MET A 259     34.242   2.358  42.237  1.00 38.48      S
ATOM  1844 CE  MET A 259     35.844   2.502  42.974  1.00 37.84      C
ATOM  1845 C   MET A 259     30.638   3.283  44.029  1.00 33.14      C
ATOM  1846 O   MET A 259     30.189   2.272  44.569  1.00 33.45      O
ATOM  1847 N   THR A 260     29.912   4.076  43.250  1.00 32.81      N
ATOM  1848 CA  THR A 260     28.509   3.827  42.955  1.00 32.55      C
ATOM  1849 CB  THR A 260     27.706   5.132  42.987  1.00 32.69      C
ATOM  1850 OG1 THR A 260     28.140   5.973  41.907  1.00 32.32      O
ATOM  1851 CG2 THR A 260     27.911   5.857  44.304  1.00 32.38      C
ATOM  1852 C   THR A 260     28.362   3.260  41.551  1.00 32.45      C
ATOM  1853 O   THR A 260     29.311   3.264  40.765  1.00 32.43      O
ATOM  1854 N   PRO A 261     27.165   2.765  41.212  1.00 32.43      N
ATOM  1855 CD  PRO A 261     26.012   2.408  42.064  1.00 32.73      C
ATOM  1856 CA  PRO A 261     27.002   2.227  39.862  1.00 32.04      C
ATOM  1857 CB  PRO A 261     25.559   1.726  39.864  1.00 32.40      C
ATOM  1858 CG  PRO A 261     25.383   1.268  41.293  1.00 32.56      C
ATOM  1859 C   PRO A 261     27.244   3.333  38.835  1.00 31.88      C
ATOM  1860 O   PRO A 261     27.850   3.096  37.796  1.00 31.83      O
ATOM  1861 N   GLY A 262     26.779   4.545  39.139  1.00 31.39      N
ATOM  1862 CA  GLY A 262     26.971   5.660  38.225  1.00 30.93      C
ATOM  1863 C   GLY A 262     28.439   5.941  37.935  1.00 30.03      C
ATOM  1864 O   GLY A 262     28.831   6.103  36.782  1.00 30.46      O
ATOM  1865 N   ALA A 263     29.254   6.003  38.980  1.00 29.43      N
ATOM  1866 CA  ALA A 263     30.678   6.248  38.816  1.00 28.87      C
ATOM  1867 CB  ALA A 263     31.342   6.409  40.178  1.00 28.90      C
ATOM  1868 C   ALA A 263     31.329   5.099  38.052  1.00 28.88      C
ATOM  1869 O   ALA A 263     32.162   5.314  37.170  1.00 28.36      O
ATOM  1870 N   GLU A 264     30.944   3.874  38.396  1.00 28.76      N
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Figure 10HH

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ATOM  1871  CA  GLU A 264      31.505   2.691  37.752  1.00 29.21      C
ATOM  1872  CB  GLU A 264      30.980   1.432  38.457  1.00 29.05      C
ATOM  1873  CG  GLU A 264      31.358   1.396  39.931  1.00 29.36      C
ATOM  1874  CD  GLU A 264      30.506   0.450  40.767  1.00 29.84      C
ATOM  1875  OE1 GLU A 264      29.389   0.097  40.345  1.00 29.77      O
ATOM  1876  OE2 GLU A 264      30.955   0.080  41.870  1.00 30.70      O
ATOM  1877  C   GLU A 264      31.187   2.662  36.258  1.00 29.35      C
ATOM  1878  O   GLU A 264      32.006   2.220  35.451  1.00 29.37      O
ATOM  1879  N   GLN A 265      30.010   3.157  35.892  1.00 29.70      N
ATOM  1880  CA  GLN A 265      29.601   3.179  34.495  1.00 30.44      C
ATOM  1881  CB  GLN A 265      28.137   3.606  34.381  1.00 31.82      C
ATOM  1882  CG  GLN A 265      27.210   2.667  35.117  1.00 35.27      C
ATOM  1883  CD  GLN A 265      25.751   3.021  34.954  1.00 37.03      C
ATOM  1884  OE1 GLN A 265      24.889   2.428  35.607  1.00 39.00      O
ATOM  1885  NE2 GLN A 265      25.459   3.984  34.078  1.00 38.41      N
ATOM  1886  C   GLN A 265      30.474   4.076  33.621  1.00 29.94      C
ATOM  1887  O   GLN A 265      30.392   4.015  32.396  1.00 29.87      O
ATOM  1888  N   LEU A 266      31.299   4.906  34.247  1.00 29.15      N
ATOM  1889  CA  LEU A 266      32.198   5.791  33.506  1.00 29.01      C
ATOM  1890  CB  LEU A 266      32.496   7.055  34.318  1.00 28.73      C
ATOM  1891  CG  LEU A 266      31.367   8.075  34.425  1.00 29.05      C
ATOM  1892  CD1 LEU A 266      31.842   9.274  35.237  1.00 28.78      C
ATOM  1893  CD2 LEU A 266      30.937   8.502  33.024  1.00 28.78      C
ATOM  1894  C   LEU A 266      33.523   5.113  33.169  1.00 28.86      C
ATOM  1895  O   LEU A 266      34.319   5.643  32.386  1.00 28.44      O
ATOM  1896  N   LEU A 267      33.757   3.939  33.751  1.00 28.56      N
ATOM  1897  CA  LEU A 267      35.010   3.232  33.533  1.00 28.80      C
ATOM  1898  CB  LEU A 267      34.943   1.824  34.133  1.00 29.49      C
ATOM  1899  CG  LEU A 267      36.275   1.073  34.136  1.00 29.76      C
ATOM  1900  CD1 LEU A 267      37.305   1.829  34.979  1.00 29.91      C
ATOM  1901  CD2 LEU A 267      36.058  -0.329  34.700  1.00 30.42      C
ATOM  1902  C   LEU A 267      35.483   3.150  32.080  1.00 28.65      C
ATOM  1903  O   LEU A 267      36.609   3.529  31.782  1.00 28.27      O
ATOM  1904  N   PRO A 268      34.635   2.655  31.161  1.00 28.76      N
ATOM  1905  CD  PRO A 268      33.250   2.185  31.327  1.00 29.21      C
ATOM  1906  CA  PRO A 268      35.058   2.559  29.759  1.00 29.10      C
ATOM  1907  CB  PRO A 268      33.849   1.920  29.074  1.00 29.23      C
ATOM  1908  CG  PRO A 268      32.695   2.343  29.937  1.00 29.74      C
ATOM  1909  C   PRO A 268      35.470   3.902  29.135  1.00 29.03      C
ATOM  1910  O   PRO A 268      36.458   3.971  28.408  1.00 28.44      O
ATOM  1911  N   VAL A 269      34.719   4.961  29.422  1.00 29.23      N
ATOM  1912  CA  VAL A 269      35.045   6.283  28.885  1.00 29.50      C
ATOM  1913  CB  VAL A 269      33.888   7.279  29.118  1.00 30.12      C
ATOM  1914  CG1 VAL A 269      34.278   8.681  28.649  1.00 31.29      C
ATOM  1915  CG2 VAL A 269      32.667   6.812  28.338  1.00 31.48      C
ATOM  1916  C   VAL A 269      36.328   6.791  29.536  1.00 29.16      C
ATOM  1917  O   VAL A 269      37.220   7.299  28.852  1.00 29.31      O
ATOM  1918  N   LEU A 270      36.438   6.635  30.853  1.00 28.36      N
ATOM  1919  CA  LEU A 270      37.640   7.062  31.547  1.00 28.07      C
ATOM  1920  CB  LEU A 270      37.531   6.749  33.048  1.00 27.79      C
ATOM  1921  CG  LEU A 270      36.555   7.621  33.858  1.00 27.73      C
ATOM  1922  CD1 LEU A 270      36.423   7.075  35.273  1.00 26.65      C
ATOM  1923  CD2 LEU A 270      37.060   9.062  33.893  1.00 27.37      C
ATOM  1924  C   LEU A 270      38.859   6.358  30.942  1.00 28.42      C
ATOM  1925  O   LEU A 270      39.918   6.968  30.759  1.00 28.07      O
ATOM  1926  N   GLN A 271      38.706   5.075  30.620  1.00 28.62      N
ATOM  1927  CA  GLN A 271      39.803   4.309  30.036  1.00 29.58      C
ATOM  1928  CB  GLN A 271      39.446   2.815  30.009  1.00 29.77      C
```

Figure 10II

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ATOM  1929  CG  GLN A 271      39.562   2.171  31.395  1.00 29.56      C
ATOM  1930  CD  GLN A 271      39.100   0.719  31.441  1.00 30.15      C
ATOM  1931  OE1 GLN A 271      39.476  -0.030  32.346  1.00 30.14      O
ATOM  1932  NE2 GLN A 271      38.276   0.322  30.480  1.00 29.92      N
ATOM  1933  C   GLN A 271      40.154   4.831  28.641  1.00 30.09      C
ATOM  1934  O   GLN A 271      41.333   4.935  28.298  1.00 30.05      O
ATOM  1935  N   ARG A 272      39.139   5.173  27.850  1.00 30.62      N
ATOM  1936  CA  ARG A 272      39.372   5.733  26.519  1.00 32.09      C
ATOM  1937  CB  ARG A 272      38.051   5.959  25.769  1.00 33.56      C
ATOM  1938  CG  ARG A 272      37.497   4.712  25.080  1.00 36.87      C
ATOM  1939  CD  ARG A 272      36.510   5.071  23.966  1.00 39.07      C
ATOM  1940  NE  ARG A 272      35.236   5.575  24.474  1.00 41.31      N
ATOM  1941  CZ  ARG A 272      34.331   4.826  25.101  1.00 42.35      C
ATOM  1942  NH1 ARG A 272      34.557   3.529  25.295  1.00 42.99      N
ATOM  1943  NH2 ARG A 272      33.201   5.372  25.538  1.00 42.53      N
ATOM  1944  C   ARG A 272      40.119   7.066  26.646  1.00 31.71      C
ATOM  1945  O   ARG A 272      40.888   7.441  25.758  1.00 31.85      O
ATOM  1946  N   TYR A 273      39.892   7.775  27.751  1.00 31.12      N
ATOM  1947  CA  TYR A 273      40.560   9.053  27.996  1.00 30.49      C
ATOM  1948  CB  TYR A 273      39.764   9.912  28.988  1.00 30.13      C
ATOM  1949  CG  TYR A 273      38.764  10.843  28.338  1.00 30.08      C
ATOM  1950  CD1 TYR A 273      37.423  10.485  28.209  1.00 30.27      C
ATOM  1951  CE1 TYR A 273      36.506  11.337  27.600  1.00 30.56      C
ATOM  1952  CD2 TYR A 273      39.165  12.084  27.840  1.00 30.11      C
ATOM  1953  CE2 TYR A 273      38.257  12.944  27.231  1.00 30.62      C
ATOM  1954  CZ  TYR A 273      36.932  12.566  27.113  1.00 31.12      C
ATOM  1955  OH  TYR A 273      36.035  13.413  26.506  1.00 31.48      O
ATOM  1956  C   TYR A 273      41.992   8.902  28.510  1.00 30.66      C
ATOM  1957  O   TYR A 273      42.738   9.878  28.577  1.00 30.68      O
ATOM  1958  N   GLY A 274      42.383   7.687  28.879  1.00 30.61      N
ATOM  1959  CA  GLY A 274      43.740   7.489  29.356  1.00 30.77      C
ATOM  1960  C   GLY A 274      43.881   7.150  30.830  1.00 31.11      C
ATOM  1961  O   GLY A 274      44.991   7.138  31.358  1.00 30.91      O
ATOM  1962  N   PHE A 275      42.766   6.888  31.503  1.00 31.47      N
ATOM  1963  CA  PHE A 275      42.810   6.527  32.918  1.00 32.19      C
ATOM  1964  CB  PHE A 275      41.801   7.348  33.728  1.00 31.21      C
ATOM  1965  CG  PHE A 275      42.032   8.831  33.653  1.00 30.69      C
ATOM  1966  CD1 PHE A 275      41.342   9.611  32.729  1.00 30.41      C
ATOM  1967  CD2 PHE A 275      42.970   9.441  34.477  1.00 29.75      C
ATOM  1968  CE1 PHE A 275      41.587  10.983  32.624  1.00 30.10      C
ATOM  1969  CE2 PHE A 275      43.223  10.809  34.382  1.00 30.33      C
ATOM  1970  CZ  PHE A 275      42.529  11.582  33.451  1.00 30.15      C
ATOM  1971  C   PHE A 275      42.471   5.048  33.007  1.00 33.19      C
ATOM  1972  O   PHE A 275      41.321   4.655  32.821  1.00 33.75      O
ATOM  1973  N   GLU A 276      43.484   4.234  33.277  1.00 34.59      N
ATOM  1974  CA  GLU A 276      43.310   2.789  33.361  1.00 36.07      C
ATOM  1975  CB  GLU A 276      44.675   2.103  33.438  1.00 37.83      C
ATOM  1976  CG  GLU A 276      45.583   2.659  34.528  1.00 39.84      C
ATOM  1977  CD  GLU A 276      46.443   1.587  35.173  1.00 41.24      C
ATOM  1978  OE1 GLU A 276      46.984   0.727  34.439  1.00 42.52      O
ATOM  1979  OE2 GLU A 276      46.588   1.607  36.415  1.00 41.91      O
ATOM  1980  C   GLU A 276      42.478   2.336  34.544  1.00 35.79      C
ATOM  1981  O   GLU A 276      41.703   1.381  34.442  1.00 35.99      O
ATOM  1982  N   THR A 277      42.632   3.035  35.662  1.00 35.29      N
ATOM  1983  CA  THR A 277      41.938   2.665  36.885  1.00 35.33      C
ATOM  1984  CB  THR A 277      42.976   2.238  37.953  1.00 35.95      C
ATOM  1985  OG1 THR A 277      43.827   1.222  37.404  1.00 37.35      O
ATOM  1986  CG2 THR A 277      42.292   1.707  39.198  1.00 36.44      C
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Figure 10JJ

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ATOM  1987 C   THR A 277    41.056  3.753 37.487  1.00 34.38      C
ATOM  1988 O   THR A 277    41.325  4.946 37.339  1.00 33.90      O
ATOM  1989 N   LEU A 278    39.999  3.309 38.162  1.00 33.42      N
ATOM  1990 CA  LEU A 278    39.063  4.180 38.860  1.00 32.84      C
ATOM  1991 CB  LEU A 278    37.660  4.078 38.261  1.00 32.25      C
ATOM  1992 CG  LEU A 278    36.557  4.754 39.080  1.00 31.65      C
ATOM  1993 CD1 LEU A 278    36.739  6.269 39.067  1.00 31.85      C
ATOM  1994 CD2 LEU A 278    35.204  4.385 38.506  1.00 32.00      C
ATOM  1995 C   LEU A 278    39.029  3.683 40.301  1.00 32.90      C
ATOM  1996 O   LEU A 278    38.696  2.523 40.551  1.00 32.50      O
ATOM  1997 N   GLU A 279    39.390  4.549 41.242  1.00 32.79      N
ATOM  1998 CA  GLU A 279    39.390  4.191 42.657  1.00 33.18      C
ATOM  1999 CB  GLU A 279    40.821  4.141 43.212  1.00 33.85      C
ATOM  2000 CG  GLU A 279    41.704  3.034 42.652  1.00 34.93      C
ATOM  2001 CD  GLU A 279    43.103  3.054 43.243  1.00 35.80      C
ATOM  2002 OE1 GLU A 279    43.990  2.345 42.711  1.00 37.17      O
ATOM  2003 OE2 GLU A 279    43.323  3.773 44.242  1.00 35.89      O
ATOM  2004 C   GLU A 279    38.596  5.205 43.472  1.00 33.21      C
ATOM  2005 O   GLU A 279    38.373  6.340 43.037  1.00 31.95      O
ATOM  2006 N   LYS A 280    38.173  4.786 44.660  1.00 33.51      N
ATOM  2007 CA  LYS A 280    37.438  5.666 45.550  1.00 34.17      C
ATOM  2008 CB  LYS A 280    36.529  4.868 46.489  1.00 34.76      C
ATOM  2009 CG  LYS A 280    35.955  5.721 47.620  1.00 35.25      C
ATOM  2010 CD  LYS A 280    34.963  4.950 48.463  1.00 36.16      C
ATOM  2011 CE  LYS A 280    34.444  5.796 49.618  1.00 36.76      C
ATOM  2012 NZ  LYS A 280    33.323  5.103 50.330  1.00 37.23      N
ATOM  2013 C   LYS A 280    38.437  6.456 46.382  1.00 34.45      C
ATOM  2014 O   LYS A 280    39.405  5.901 46.896  1.00 34.38      O
ATOM  2015 N   LEU A 281    38.204  7.756 46.503  1.00 34.75      N
ATOM  2016 CA  LEU A 281    39.079  8.605 47.293  1.00 35.65      C
ATOM  2017 CB  LEU A 281    39.370  9.908 46.550  1.00 35.08      C
ATOM  2018 CG  LEU A 281    40.280 10.898 47.278  1.00 34.82      C
ATOM  2019 CD1 LEU A 281    41.691 10.337 47.360  1.00 34.07      C
ATOM  2020 CD2 LEU A 281    40.273 12.230 46.537  1.00 34.40      C
ATOM  2021 C   LEU A 281    38.392  8.920 48.618  1.00 36.70      C
ATOM  2022 O   LEU A 281    37.230  9.325 48.635  1.00 36.57      O
ATOM  2023 N   ALA A 282    39.105  8.726 49.722  1.00 37.88      N
ATOM  2024 CA  ALA A 282    38.551  9.008 51.045  1.00 39.41      C
ATOM  2025 CB  ALA A 282    39.297  8.204 52.111  1.00 39.19      C
ATOM  2026 C   ALA A 282    38.687 10.501 51.327  1.00 40.14      C
ATOM  2027 O   ALA A 282    39.798 11.023 51.394  1.00 40.34      O
ATOM  2028 N   VAL A 283    37.556 11.179 51.500  1.00 41.23      N
ATOM  2029 CA  VAL A 283    37.550 12.617 51.757  1.00 42.40      C
ATOM  2030 CB  VAL A 283    36.640 13.340 50.746  1.00 42.15      C
ATOM  2031 CG1 VAL A 283    36.654 14.834 51.008  1.00 42.12      C
ATOM  2032 CG2 VAL A 283    37.097 13.037 49.330  1.00 42.22      C
ATOM  2033 C   VAL A 283    37.073 12.974 53.168  1.00 43.56      C
ATOM  2034 O   VAL A 283    36.188 12.315 53.718  1.00 43.82      O
ATOM  2035 N   LEU A 284    37.658 14.025 53.743  1.00 44.69      N
ATOM  2036 CA  LEU A 284    37.290 14.488 55.084  1.00 45.88      C
ATOM  2037 CB  LEU A 284    38.534 14.635 55.968  1.00 46.17      C
ATOM  2038 CG  LEU A 284    39.537 13.487 56.073  1.00 46.66      C
ATOM  2039 CD1 LEU A 284    40.567 13.830 57.143  1.00 46.97      C
ATOM  2040 CD2 LEU A 284    38.822 12.191 56.420  1.00 46.95      C
ATOM  2041 C   LEU A 284    36.591 15.844 55.006  1.00 46.59      C
ATOM  2042 O   LEU A 284    36.980 16.790 55.699  1.00 47.10      O
ATOM  2043 N   GLY A 285    35.567 15.945 54.165  1.00 47.04      N
ATOM  2044 CA  GLY A 285    34.858 17.204 54.025  1.00 47.76      C
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Figure 10KK

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ATOM  2045  C   GLY A 285     33.866  17.240  52.875  1.00 47.90      C
ATOM  2046  O   GLY A 285     32.783  17.840  53.035  1.00 48.58      O
ATOM  2047  OXT GLY A 285     34.176  16.690  51.803  1.00 48.12      O
ATOM  2107  OH2 WAT S   1     28.597  26.858  34.170  1.00 35.33      O
ATOM  2108  OH2 WAT S   2     39.874  15.622  52.951  1.00 27.02      O
ATOM  2109  OH2 WAT S   3     47.806  29.582  41.793  1.00 26.82      O
ATOM  2110  OH2 WAT S   4     32.712  12.071  49.955  1.00 33.48      O
ATOM  2111  OH2 WAT S   5     34.388  29.141  28.290  1.00 23.66      O
ATOM  2112  OH2 WAT S   6     29.860  12.057  36.929  1.00 28.75      O
ATOM  2113  OH2 WAT S   7     18.596  31.078  31.314  1.00 34.56      O
ATOM  2114  OH2 WAT S   8     43.746  30.135  36.454  1.00 31.70      O
ATOM  2115  OH2 WAT S   9     40.710  28.228  24.786  1.00 32.34      O
ATOM  2116  OH2 WAT S  10     40.249  20.233  54.144  1.00 31.31      O
ATOM  2117  OH2 WAT S  11     50.729  22.205  49.175  1.00 29.78      O
ATOM  2118  OH2 WAT S  12     36.244  25.185  28.517  1.00 31.80      O
ATOM  2119  OH2 WAT S  13     29.586   1.690  31.020  1.00 35.67      O
ATOM  2120  OH2 WAT S  14     27.347   8.426  41.609  1.00 33.85      O
ATOM  2121  OH2 WAT S  15     37.753  30.653  48.262  1.00 31.49      O
ATOM  2122  OH2 WAT S  16     39.852   0.508  38.143  1.00 34.51      O
ATOM  2123  OH2 WAT S  17     49.787  10.549  30.555  1.00 37.19      O
ATOM  2124  OH2 WAT S  18     48.590  27.775  45.618  1.00 37.05      O
ATOM  2125  OH2 WAT S  19     46.426  30.341  36.837  1.00 31.78      O
ATOM  2126  OH2 WAT S  20     26.420  26.789  43.445  1.00 49.61      O
ATOM  2127  OH2 WAT S  21     46.268  30.739  29.048  1.00 36.68      O
ATOM  2128  OH2 WAT S  22     51.867  28.804  43.136  1.00 49.35      O
ATOM  2129  OH2 WAT S  23     36.825  15.509  25.141  1.00 33.48      O
ATOM  2130  OH2 WAT S  24     33.895  12.303  25.137  1.00 32.90      O
ATOM  2131  OH2 WAT S  25     36.781  35.492  29.625  1.00 32.04      O
ATOM  2132  OH2 WAT S  26     33.992  25.683  29.926  1.00 34.00      O
ATOM  2133  OH2 WAT S  27     24.645  23.077  49.434  1.00 37.03      O
ATOM  2134  OH2 WAT S  28     37.658  21.847  53.629  1.00 28.23      O
ATOM  2135  OH2 WAT S  29     43.589  10.679  50.593  1.00 35.31      O
ATOM  2136  OH2 WAT S  30     23.719  24.494  52.323  1.00 35.79      O
ATOM  2137  OH2 WAT S  31     39.337  10.396  24.048  1.00 52.48      O
ATOM  2138  OH2 WAT S  32     30.718  16.193  20.614  1.00 43.40      O
ATOM  2139  OH2 WAT S  33     54.666   8.115  42.921  1.00 47.38      O
ATOM  2140  OH2 WAT S  34     31.589  30.437  35.873  1.00 47.91      O
ATOM  2141  OH2 WAT S  35     50.340  32.089  31.165  1.00 41.42      O
ATOM  2142  OH2 WAT S  36     52.796  22.874  51.515  1.00 43.37      O
ATOM  2143  OH2 WAT S  37     55.373  22.792  30.536  1.00 57.15      O
ATOM  2144  OH2 WAT S  38     39.463  35.817  35.231  1.00 32.47      O
ATOM  2145  OH2 WAT S  39     16.092  27.159  27.724  1.00 37.21      O
ATOM  2146  OH2 WAT S  40     25.640  24.780  14.005  1.00 45.10      O
ATOM  2147  OH2 WAT S  41     50.761   2.536  38.098  1.00 52.36      O
ATOM  2148  OH2 WAT S  42     18.634  34.668  30.052  1.00 43.13      O
ATOM  2149  OH2 WAT S  43     38.535  -2.076  28.925  1.00 32.09      O
ATOM  2150  OH2 WAT S  44     13.196  24.012  19.544  1.00 39.80      O
ATOM  2151  OH2 WAT S  45     31.357  26.426  13.729  1.00 42.37      O
ATOM  2152  OH2 WAT S  46     52.281  28.184  27.760  1.00 36.04      O
ATOM  2153  OH2 WAT S  47     46.418  33.201  38.411  1.00 44.49      O
ATOM  2154  OH2 WAT S  48     53.339  19.767  45.907  1.00 33.06      O
ATOM  2155  OH2 WAT S  49     46.967  16.612  52.076  1.00 30.83      O
ATOM  2156  OH2 WAT S  50     36.971  22.531  27.836  1.00 27.70      O
ATOM  2157  OH2 WAT S  51     34.404  33.315  13.713  1.00 63.94      O
ATOM  2158  OH2 WAT S  52     25.500  12.910  42.366  1.00 44.85      O
ATOM  2159  OH2 WAT S  53     41.068  33.656  19.666  1.00 61.38      O
ATOM  2160  OH2 WAT S  54     47.085  26.379  21.851  1.00 40.28      O
ATOM  2161  OH2 WAT S  55     20.530  37.341  28.713  1.00 42.17      O
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Figure 10LL

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ATOM  2162 OH2 WAT S  56      45.303  21.686  23.767  1.00 31.71           O
ATOM  2163 OH2 WAT S  57      32.171   3.766  47.945  1.00 39.12           O
ATOM  2164 OH2 WAT S  58      29.040  34.613  43.652  1.00 54.88           O
ATOM  2165 OH2 WAT S  59      63.169  17.639  43.696  1.00 51.86           O
ATOM  2166 OH2 WAT S  60      17.466  39.005  16.986  1.00 43.71           O
ATOM  2167 OH2 WAT S  61      31.214   5.360  30.303  1.00 35.40           O
ATOM  2168 OH2 WAT S  62      32.083  34.301  14.884  1.00 43.78           O
ATOM  2169 OH2 WAT S  63      56.027  25.650  46.067  1.00 55.28           O
ATOM  2170 OH2 WAT S  64      49.021  30.852  29.187  1.00 36.47           O
ATOM  2171 OH2 WAT S  65      23.639  30.939  17.071  1.00 45.30           O
ATOM  2172 OH2 WAT S  66      37.468  39.280  36.056  1.00 51.85           O
ATOM  2173 OH2 WAT S  67      36.224  28.879  18.295  1.00 42.91           O
ATOM  2174 OH2 WAT S  68      24.175  22.019  37.073  1.00 26.31           O
ATOM  2175 OH2 WAT S  69      22.152  26.896  48.344  1.00 61.11           O
ATOM  2176 OH2 WAT S  70      48.970   6.753  46.837  1.00 48.46           O
ATOM  2177 OH2 WAT S  71      42.273  27.745  52.837  1.00 33.63           O
ATOM  2178 OH2 WAT S  72      53.543  28.612  47.788  1.00 36.22           O
ATOM  2179 OH2 WAT S  73       8.907  23.447  21.629  1.00 50.44           O
ATOM  2180 OH2 WAT S  74      34.479  41.295  17.726  1.00 40.28           O
ATOM  2181 OH2 WAT S  75      34.584  20.083  21.656  1.00 47.04           O
ATOM  2182 OH2 WAT S  76      48.365   7.218  39.795  1.00 37.47           O
ATOM  2183 OH2 WAT S  77      17.856  23.193  14.949  1.00 36.50           O
ATOM  2184 OH2 WAT S  78      22.607  24.686  38.024  1.00 40.25           O
ATOM  2185 OH2 WAT S  79      21.034  18.474  37.563  1.00 57.62           O
ATOM  2186 OH2 WAT S  80      52.538   9.289  46.345  1.00 43.42           O
ATOM  2187 OH2 WAT S  81      29.673  13.056  39.115  1.00 28.10           O
ATOM  2188 OH2 WAT S  82      25.423  30.052  47.729  1.00 43.44           O
ATOM  2189 OH2 WAT S  83      27.721  18.627  14.255  1.00 44.64           O
ATOM  2190 OH2 WAT S  84      59.509  32.103  35.721  1.00 63.08           O
ATOM  2191 OH2 WAT S  85      44.482  33.024  48.358  1.00 36.03           O
ATOM  2192 OH2 WAT S  86      41.973   7.788  49.345  1.00 50.35           O
ATOM  2193 OH2 WAT S  87      37.663  22.110  25.265  1.00 41.24           O
ATOM  2194 OH2 WAT S  88      25.957  12.097  36.912  1.00 36.00           O
ATOM  2195 OH2 WAT S  89      30.437  33.017  13.345  1.00 48.23           O
ATOM  2196 OH2 WAT S  90      37.438  31.243  38.851  1.00 49.55           O
ATOM  2197 OH2 WAT S  91      19.458  34.402  26.135  1.00 43.19           O
ATOM  2198 OH2 WAT S  92      58.475  14.110  43.025  1.00 52.43           O
ATOM  2199 OH2 WAT S  93      22.370  12.343  33.413  1.00 38.81           O
ATOM  2200 OH2 WAT S  94      40.451  32.550  14.618  1.00 58.82           O
ATOM  2201 OH2 WAT S  95      54.156  16.243  28.025  1.00 48.89           O
ATOM  2202 OH2 WAT S  96      12.252  20.214  20.621  1.00 44.94           O
ATOM  2203 OH2 WAT S  97      23.229  23.360  11.991  1.00 68.77           O
ATOM  2204 OH2 WAT S  98      13.653  34.410  21.575  1.00 50.48           O
ATOM  2205 OH2 WAT S  99      29.882  16.048  51.774  1.00 53.76           O
ATOM  2206 OH2 WAT S 100      34.851   9.916  49.548  1.00 36.26           O
ATOM  2207 OH2 WAT S 101      19.731  39.777  18.001  1.00 49.92           O
ATOM  2208 OH2 WAT S 102      32.811  27.414  53.799  1.00 52.41           O
ATOM  2209 OH2 WAT S 103      54.958  10.260  45.018  1.00 61.62           O
ATOM  2210 OH2 WAT S 104      26.795   8.100  24.207  1.00 39.76           O
ATOM  2211 OH2 WAT S 105      39.473  25.414  23.627  1.00 33.71           O
ATOM  2212 OH2 WAT S 106      42.444  29.282  22.951  1.00 55.44           O
ATOM  2213 OH2 WAT S 107      54.310   2.465  42.338  1.00 81.43           O
ATOM  2214 OH2 WAT S 108      32.145  22.002  57.937  1.00 69.67           O
ATOM  2215 OH2 WAT S 109      41.182  36.953  24.858  1.00 30.32           O
ATOM  2216 OH2 WAT S 110      51.408  18.218  47.152  1.00 39.60           O
ATOM  2217 OH2 WAT S 111      31.229  18.063  15.169  1.00 58.09           O
ATOM  2218 OH2 WAT S 112      47.275  32.201  26.136  1.00 75.84           O
ATOM  2219 OH2 WAT S 113      48.484  -3.729  34.355  1.00 49.03           O
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Figure 10MM

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ATOM  2220 OH2 WAT S 114    17.441  23.890  30.338  1.00 38.38      O
ATOM  2221 OH2 WAT S 115    23.853  34.456  13.715  1.00 61.47      O
ATOM  2222 OH2 WAT S 116    22.764  12.193  26.654  1.00 52.95      O
ATOM  2223 OH2 WAT S 117    23.980  15.802  45.364  1.00 50.14      O
ATOM  2224 OH2 WAT S 118    35.972  34.774  45.163  1.00 60.33      O
ATOM  2225 OH2 WAT S 119    37.807  19.398  24.708  1.00 61.62      O
ATOM  2226 OH2 WAT S 120    18.366  12.430  18.822  1.00 41.37      O
ATOM  2227 OH2 WAT S 121    28.690  28.104  42.174  1.00 64.02      O
ATOM  2228 OH2 WAT S 122    49.307   6.503  32.285  1.00 36.36      O
ATOM  2229 OH2 WAT S 123    43.722   4.110  29.378  1.00 44.89      O
ATOM  2230 OH2 WAT S 124    26.343  29.966   7.876  1.00 62.82      O
ATOM  2231 OH2 WAT S 125    16.563  15.951  28.970  1.00 51.98      O
ATOM  2232 OH2 WAT S 126    20.175  23.841  38.565  1.00 55.56      O
ATOM  2233 OH2 WAT S 127    20.576  26.542  40.567  1.00 46.61      O
ATOM  2234 OH2 WAT S 128    40.494  17.605  54.649  1.00 38.00      O
ATOM  2235 OH2 WAT S 129    32.794  26.121  16.217  1.00 40.24      O
ATOM  2236 OH2 WAT S 130    32.054  30.620  12.330  1.00 41.15      O
ATOM  2237 OH2 WAT S 131    24.132   9.866  33.561  1.00 38.41      O
ATOM  2238 OH2 WAT S 132    39.539  30.733  24.819  1.00 33.26      O
ATOM  2239 OH2 WAT S 133    29.283   9.374  37.492  1.00 32.82      O
ATOM  2240 OH2 WAT S 134    27.129  12.130  39.369  1.00 36.01      O
ATOM  2241 OH2 WAT S 135    16.237  13.797  27.208  1.00 39.89      O
ATOM  2242 OH2 WAT S 136    35.590  17.878  24.571  1.00 35.55      O
ATOM  2243 OH2 WAT S 137    22.902  19.820  36.431  1.00 38.01      O
ATOM  2244 OH2 WAT S 138    52.919  12.766  42.677  1.00 32.51      O
ATOM  2245 OH2 WAT S 139    30.240  31.220  40.494  1.00 52.62      O
ATOM  2246 OH2 WAT S 140    37.369  27.649  21.696  1.00 36.64      O
ATOM  2247 OH2 WAT S 141    42.712   1.260  30.209  1.00 50.21      O
ATOM  2248 OH2 WAT S 142    24.778   5.524  41.136  1.00 37.52      O
ATOM  2249 OH2 WAT S 143    49.022  30.149  44.178  1.00 39.81      O
ATOM  2250 OH2 WAT S 144    44.239  27.252  54.601  1.00 45.46      O
ATOM  2251 OH2 WAT S 145    34.188  24.808  21.734  1.00 47.86      O
ATOM  2252 OH2 WAT S 146    32.237  13.936  23.957  1.00 47.59      O
ATOM  2253 OH2 WAT S 147    24.826  31.905  13.806  1.00 57.46      O
ATOM  2254 OH2 WAT S 148    35.287  19.774  55.093  1.00 53.61      O
ATOM  2255 OH2 WAT S 149    37.524  19.283  55.693  1.00 45.09      O
ATOM  2256 OH2 WAT S 150    35.302   8.641  24.481  1.00 51.58      O
ATOM  2257 OH2 WAT S 151    59.678  21.694  39.012  1.00 57.80      O
ATOM  2258 OH2 WAT S 152    36.143  -0.978  27.333  1.00 48.54      O
ATOM  2259 OH2 WAT S 153    14.265  20.928  14.183  1.00 62.49      O
ATOM  2260 OH2 WAT S 154    23.418  29.667  49.908  1.00 54.71      O
ATOM  2261 OH2 WAT S 155    38.604  24.411  54.120  1.00 52.33      O
ATOM  2262 OH2 WAT S 156    27.339  19.921  12.078  1.00 61.52      O
ATOM  2263 OH2 WAT S 157    55.513  12.418  43.797  1.00 48.44      O
ATOM  2264 OH2 WAT S 158    41.570  30.546  53.130  1.00 44.74      O
ATOM  2265 OH2 WAT S 159    30.332   6.416  25.709  1.00 48.89      O
ATOM  2266 OH2 WAT S 160    39.099  33.676  39.711  1.00 61.97      O
ATOM  2267 OH2 WAT S 161    25.263   8.969  43.752  1.00 53.20      O
ATOM  2268 OH2 WAT S 162    38.420  33.913  42.190  1.00 50.80      O
ATOM  2269 OH2 WAT S 163    41.309  37.709  36.508  1.00 59.09      O
ATOM  2270 OH2 WAT S 164    39.795  36.567  20.290  1.00 53.69      O
ATOM  2271 OH2 WAT S 165    17.433  22.843  32.869  1.00 39.36      O
ATOM  2272 OH2 WAT S 166    37.147   1.819  26.855  1.00 35.01      O
ATOM  2273 OH2 WAT S 167    26.808  29.856  51.140  1.00 34.22      O
ATOM  2274 OH2 WAT S 168    20.735  23.758  11.662  1.00 55.01      O
ATOM  2275 OH2 WAT S 169    37.554  20.226  20.434  1.00 54.40      O
ATOM  2276 OH2 WAT S 170    36.378  37.998  37.846  1.00 58.07      O
ATOM  2277 OH2 WAT S 171    18.421  12.604  25.862  1.00 45.72      O
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